Hendrik Heinz

Professor
Department of Chemical and Biological Engineering
University of Colorado-Boulder · Boulder, CO 80303-0596, USA
voice: +1.303.735.7517 · fax: +1.303.492.8425 · email: hendrik.heinz@colorado.edu
Web: http://www.colorado.edu/chbe/hendrik-heinz

Education

- Air Force Research Laboratory, Wright-Patterson Air Force Base, OH — 08/2006
  Postdoctoral
  Advisors: Richard A. Vaia and Barry L. Farmer
- ETH Zurich, Switzerland — 06/2003
  Ph.D. in Materials Science and Engineering
  Advisors: Ulrich W. Suter, ETH Zurich, and Kurt Binder, U Mainz

  M.Sc. (Diploma) in Chemistry — 09/2000
  Advisor: Ulrich W. Suter, ETH Zurich, and Epameinondas Leontidis, U Cyprus
- University of Heidelberg, Germany — 09/1997
  B.Sc. (Prediploma) in Chemistry

Honors and Awards

- IAAM Scientist Medal — 2024
- NASA Group Achievement Award (US-COMP) — 2023
- Amazon Scholar — 2022
- Guest Professor at Université de Paris Cité — 2022
- Fellow of the International Association for Advanced Materials (IAAM) — 2020
- Guest Professor at Université de Paris — 2020
- Outstanding Mentor Award, CU Boulder (Office of Postdoctoral Affairs) — 2018
- National Science Foundation Special Creativity Award — 2018
- Fellow of the Royal Society of Chemistry — 2016
- Sandmeyer Award, Swiss Chemical Society — 2016
- Guest Professor at International Center for Materials Nanoarchitectonics (MANA), Tsukuba, Japan — 2014
- Max Hey Medal, Mineralogical Society of UK and Ireland — 2013
- George Brown Lectureship, Mineralogical Society (Euroclay 2011) — 2011
- Guest Professor at ETH Zurich — 2011
- National Science Foundation Career Award — 2010
- Giovanni Novelli Prize, Italian Clay Group (14th Int. Clay Conf.) — 2009
- Hewlett-Packard Outstanding Junior Faculty Award, ACS COMP Division — 2006
- Member of "AFOSR Star Team" — 2005
- Graduate Scholarship of the German National Academic Foundation — 2001−2003
- Fellow of Studienstiftung des Deutschen Volkes (German Natl. Acad. Found.) — 1995−2000

- Silver medal at the 26. International Chemistry Olympiad, Oslo, Norway 1994

Internal to University of Colorado at Boulder

- Chair's Faculty Fellowship (Chemical and Biological Engineering Dept.) 2018

Appointments

- Professor 08/2021 – present
  University of Colorado, Boulder · Department of Chemical and Biological Engineering · Materials Science and Engineering Program
- Senior Editor, American Chemical Society 04/2021 – present
  (Langmuir)
- Amazon Scholar (Senior Principal Scientist, full time) 08/2022 – 2023
  Amazon · Grand Challenge Organization and AWS
- Consultant (Senior Principal Scientist, part time), Amazon 10/2021 – 07/2022
  Amazon · Grand Challenge Organization and AWS
- Associate Editor, Royal Society of Chemistry/CNRS 10/2017 – 03/2021
  (New Journal of Chemistry)
- Associate Editor, Royal Society of Chemistry 10/2015 – 10/2017
  (RSC Advances)
- Associate Professor 08/2015 – 08/2021
  University of Colorado, Boulder · Department of Chemical and Biological Engineering · Materials Science and Engineering Program
- Associate Professor 09/2012 – 08/2015
  University of Akron, Ohio · Department of Polymer Engineering
- Assistant Professor 09/2006 – 08/2012
  University of Akron, Ohio · Department of Polymer Engineering
- Postdoc (see details under education) 02/2004 – 08/2006
  Air Force Research Laboratory · WPAFB, Ohio
- Research Associate 09/2003 – 01/2004
  ETH Zurich and Sika AG · Zurich · Switzerland

Publications in Peer-Reviewed Journals and Book Chapters

H index 62, >15,000 citations (Google Scholar), Researcher ID: E-3866-2010
Annotations: * = Invited, (*) = Corresponding authors, & = student is one of the authors
GS = grad student, PD = postdoc, UGS = undergraduate student

Highest cited first author publications: >1250 for #16, >1150 for #45, >690 for #68

Papers in Preparation (selected) and Under Review

156. "Real-Time Prediction of Perovskite Dimensionality from the Chemical Composition Using Crystallographic Databases and Machine Learning"
Isaac Armstrong, Paulina Apanel, William Ashcraft, Migon Choi, David Mitzi, Seth Marder, Hendrik Heinz
(in preparation)

155. "Force Field Parameters for Lithium Cobalt Oxide and Multiphase Battery Materials"
Liu, J. (PD); Cui, Q.; **Heinz, H.** (*) &
(submitted)

154. "Understanding the Effect of Peptides Adsorbed on Hydroxyapatite Surface on Shape and Mineralization Control by Molecular Dynamic Simulation"
Liu, J. (PD); Hoff, S. E. (GS); VanOsten, S. K.; Boone, K.; Pramanik, C. (PD); Jamil, T. (GS); Tamerler, C.; **Heinz, H.** (*) &
(submitted)

153. "INTERFACE Force Field Parameter for Inorganic/Organic Perovskites in Beyond-DFT Accuracy"
Leo Beck, Barbara Morales, Isaac Armstrong, Hendrik Heinz
(in preparation)

152. "Biphenylene AlN: An Exceptionally High-Performance Nanosheet for Green Hydrogen Storage"
Muhammad Huzaifa; Muhammad Shafiq; Afsheen Razzaq; Hendrik Heinz; Mohammad Nur-e-Alam; Tawfeq A AlHowiriny; Ul-Haq, Zaheer
(submitted)

151. "Enhancing Dimensionality Prediction in Hybrid Metal Halides via Feature Engineering and Class-Imbalance Mitigation"
Karabin, M; Armstrong, I. W. (GS); Beck, L. (GS); Apanel, P. (UG); Eisenbach. M.; Mitzi, D. B.; Terletska, H.; Heinz, H. (*)&
(submitted)

150. "INTERFACE Force Field for Alumina with Validated Bulk Phases and a pH-Resolved Surface Model Database for Electrolyte and Organic Interfaces"
Zhu, C. (PD); Kanhaiya, K. (GS); Darouich, S.; Florez, S. P. (GS); Sen, K.; Keil, P.; Khelfallah, N. S.; Schreiner, E.; Mishra, R. K. (*); **Heinz, H.** (*) &
(submitted)

149. "Substrate-Directed Dimensional and Phase Control of Peptide Assemblies on Two-Dimensional van der Waals Materials"
Xia, Ying Kim, Seonghan; Zhang, Mingyi; Lin, Yueai; Zhang, Shuai; Zhao, Yuzhou; Liu, Jun; Jin, Song; Heinz, Hendrik; Im, Wonpil; De Yoreo, James
(in revision)

148. "Validated Reactive Force Field Quantifies MXene Interfacial Properties, Mechanics, and

Thermal Transport"
Armstrong, I. W. (GS); Slocik, J. M.; Beck, L. (GS); Nepal, D.; Zhu, C. (PD); Varshney, V.; Heinz, H. (*)&
(in revision)

147. "Design Principles for Ionic Liquids in Carbon Capture Revealed by an Interpretable Chemical Force Field"
Armstrong, I. W. (GS), Kurani, S. (UG); Zhu, C. (PD); Nabity, J.; Heinz, H. (*) &
(in revision)

Published/Accepted

146. "Genetically Engineered Peptides for the Biomimetic Mineralisation of Metal-Organic Frameworks"
Lymperopoulou, S.; Hoff, S. (GS); Sola-Rabada, A.; Michaelis, M.; Efimov, I.; Westcott, Z. C.; Willimott, I. J.; Chiacchia, M.; **Heinz, H.** (*); Perry, C. C.; Bradshaw, D.
Chem 2026 (accepted). (IF 20)

145. "Unveiling the Quantum Capacitance of Zr3C2T2 (T= O, F) for High-Performance Zn-ion Hybrid Supercapacitors"
Huzaifa, M.; Ali, M.; Mahsud, A.; Nur-e-Alam, M.; Heinz, H.; Ul-Haq, Z.
J. Power Sources 2026, 666, 239039. DOI: 10.1016/j.jpowsour.2025.239039 (IF 8)

144. "Li-Functionalized Hexagonal Boron Trioxide (h-B2O3) Nanosheets: A High-Performance Sustainable Hydrogen Storage Solution"
Ali, M.; Huzaifa, M.; Razzaq, A.; Heinz, H; Nur-e-Alam, M.; Ul-Haq, Z.
J. Energy Storage 2025, 140, 118555. DOI: 10.1016/j.est.2025.118555 (IF 9.8)

143. "Unveiling Ligand-Induced Conformational Changes in Mutant AR-LBD: Molecular Dynamics Insights into Androgen Receptor-Coactivator Mechanism"
Sardar, M.; Ahmad, N.; Mushtaq, M.; Heinz, H.; Nur-e-Alam, M.; Ul-Haq, Z.
J. Chem. Inf. Model. 2025, 65, 9154-9176. DOI: 10.1021/acs.jcim.5c01406 (IF 5.3)

142. "Integrating Complete Bond Dissociation in Class II Force Fields"
Kemppainen, J.; Heinz, H., Odegard, G.
NPJ Comput. Mater. 2025, 11, 341. DOI: 10.1038/s41524-025-01838-5 (IF 12)

141. "Molecular Insights into the Role of Estrogen Receptor Beta in Ecdysterone Mediated Anabolic Activity"
Tariq, S. S.; Sahar, M.; Shafiq, M.; Heinz, H.; Nur-e-Alam, M.; Ahmed, A.; Ul-Haq, Z.
PLoS One 2025, 20, e0320865. DOI: 10.1371/journal.pone.0320865 (IF 3.2)

140. "Towards MatCore: A Unified Metadata Standard for Materials Science"
Greenberg, J.; Bóveda-Aguirre, P.; Allison, J.; Asinari, P.; Chan, M.; Chandrasekaran, A.; Ertekin, E.; Garoufallou, E.; Galli, G.; Giannozzi, P.; Giustino, F.; Goldbeck, G.; Heinz, H.; Jayaraman, A.; Lordi, V.; Persson, K. A.; Rignanese, G.-M.; Thompson, A.; Toberer, E.; McClellan, S.; Tadmor, E. B. In *Metadata and Semantic Research. MTSR*

2024. Communications in Computer and Information Science, Vol 2331, Cham, Springer Nature Switzerland: Cham, 2025; pp 3-14. DOI: 10.1007/978-3-031-81974-2_1

139. "Prediction of Carbon Nanostructure Mechanical Properties and the Role of Defects Using Machine Learning"
Winetrout, J. J. (GS); Li, Z.; Zhao, Q.; Gaber, L.; Unnikrishnan, V. U.; Varshney, V.; Xu, Y.; Wang, Y. (*); **Heinz, H.** (*) &
Proc. Natl. Acad. Sci. USA 2025, 122, e2415068122. DOI: 10.1073/pnas.2415068122. (IF 10)

138. "Dataset of Carbon Nanostructures for "Prediction of Carbon Nanostructure Mechanical Properties and the Role of Defects Using Machine Learning""
Winetrout, J. J. (GS); Li, Z.; Zhao, Q.; Gaber, L.; Unnikrishnan, V. U.; Varshney, V.; Xu, Y.; Wang, Y. (*); **Heinz, H.** (*) &
Figshare 2025: DOI: 10.6084/m9.figshare.27634290. (2000+ structures with properties)

137. "Understanding Hydration Reactions, Mechanical Properties, Thermal Expansion, and Organic Interfacial Interactions of Calcium Sulfate Hydrates from the Atomic Scale"
Mishra, R. K. (GS); Darouich, S.; in 't Veld, P. J.; Flatt, R. J. (*); **Heinz, H**. (*) &
Cem. Concr. Res. 2025, 189, 107740. DOI: 10.1016/j.cemconres.2024.107740 (IF 11)

136. "Atomic-Scale Identification of the Active Sites of Nanocatalysts"
Yang, Y.; Zhou, J.; Zhao, Z.; Sun, G.; Ophus, C.; Moniri, S.; Yang, Y.; Wei, Z.; Yuan, Y.; Zhu, C. (PD); Jia, Q.; Heinz, H.; Ciston, J.; Sautet, P.; Ercius, P.; Huang, Y.; Miao, J.
Nat. Catal. 2024, 7, 796-806. DOI: 10.1038/s41929-024-01175-8 (IF 41)

135. "Surface Molecular Pump Enables Ultrahigh Catalyst Activity"
Huang, J.; Peng, B.; Zhu, C. (PD); Xu, M.; Liu, Z.; Duan, X.; **Heinz, H.** (*); Huang, Y. (*)
Sci. Adv. 2024, 10, ado3942. DOI: 10.1126/sciadv.ado3942. (IF 14)

134. „Implementing Reactivity in Molecular Dynamics Simulations with Harmonic Force Fields"
Winetrout, J. J. (GS); Kanhaiya, K. (GS); Sachdeva, G.; Pandey, R.; Damirchi, B.; Van Duin, A.; Odegard, G. M.; **Heinz, H.** (*) &
Nat. Comm. 2024, 15, 7945. DOI: 10.1038/s41467-024-50793-0. (IF 16)

133. "Type Label Framework for Bonded Force Fields in LAMMPS: OpenKIM Archiving, Testing, and Usage"
Gissinger, J.; Nikiforov, I.; Afshar, Y.; Waters, B.; Choi, M.-K.; Karls, D.; Stukowski, A.; Im, W.; Heinz, H.; Kohlmeyer, A.; Tadmor, E.
J. Phys. Chem. B 2024, 128, 3282-3297. DOI: 10.1021/acs.jpcb.3c08419 (IF 2.8)

132.*"Osteocalcin: Promoter or Inhibitor of Hydroxyapatite Growth?"
Tavakol, M. (GS/PD); Liu, J. (PD); Hoff, S. E. (GS); Zhu, C. (PD); Heinz, H. (*) &
Langmuir 2024, 40, 1747-1760. DOI: acs.langmuir.3c02948 (IF 4)

131. "Analyzing the Li–Al–O Interphase of Atomic Layer-Deposited Al2O3 Films on Layered Oxide Cathodes Using Atomistic Simulations"

Ngyuyen, J. A. (GS); Becker, A. (UGS); Kanhaiya, K. (GS); Heinz, H. (*); Weimer, A. W. (*) &
ACS Appl. Mater. Interfaces 2024, 16, 1861-1875. DOI: 10.1021/acsami.3c15080 (IF 9.5)

130. "Accurate Force Fields for Atomistic Simulations of Oxides, Hydroxides, and Organic Hybrid Materials up to the Micrometer Scale"
Kanhaiya, K. (GS); Nathanson, M. (GS); in 't Veld, P. J.; Zhu, C. (PD); Nikiforov, I.; Tadmor, E. B.; Choi, Y. K.; Im, W.; Mishra, R. K.; Heinz, H. (*) &
J. Chem. Theor. Comput. 2023, 19, 8293-8322. DOI: 10.1021/acs.jctc.3c00750 (IF 5.5)

129.*"2023 Highlights in Interface Science and Engineering: A Collection of Virtual Special Issues"
Heinz, H.; Joshi, Y. M.; Zeng, H.; Tsao, H.-K.; de Beer, S. J. A.; Koos, E.; Takahara, A.; Walker, G. C.
Langmuir 2023, 39, 10711-10714. DOI: 10.1021/acs.langmuir.3c01562 (IF 4)

128. "Accurate and Ultrafast Simulation of Molecular Recognition and Assembly on Metal Surfaces in Four Dimensions"
Zhu, C. (PD); Hoff, S. E. (GS); Hemadi, M.; **Heinz, H.** (*) &
ACS Nano 2023, 17, 9938-9952. DOI: 10.1021/acsnano.2c10953 (IF 18)

127. „Voltage Modulated Untwist Deformations and Multispectral Optical Effects from Ion Intercalation into Chiral Ceramic Nanoparticles"
Shao, X.; Zhu, C. (PD); Kumar, P.; Wang, Y.; Lu, J.; Cha, M., Yao, L.; Cao, Y.; Mao, X.; Heinz, H. (*), Kotov, N. A. (*) &
Adv. Mater. 2023, 35, 2370116. DOI: 10.1002/adma.202206956 (IF 30)

126. "Boron Nitride Nanotubes: Force Field Parameterization, Epoxy Interactions, and Comparison with Carbon Nanotubes for High-Performance Composite Materials"
Bamane, S. S.; Jakubinek, M. B.; Kanhaiya, K. (GS); Ashrafi, B.; Heinz, H.; Odegard, G. M.
ACS Appl. Nano Mater. 2023, 6, 3513-3524. DOI: 10.1021/acsanm.2c05285 (IF 5.9).

125.*"Hierarchically Structured Bioinspired Nanocomposites"
Nepal, D.(*); Kang, S.; Adstedt, K. M.; Kanhaiya, K. (GS); Bockstaller, M. R.; Brinson, L. C.; Buehler, M. J.; Coveney, P. V.; Dayal, K.; El-Awady, J. A.; Henderson, L. C.; Kaplan, D. L.; Keten, S.; Kotov, N. A.; Schatz, G. C.; Vignolini, S.; Vollrath, F.; Wang, Y.; Yacobson, B. I.; Tsukruk, V. V.(*); Heinz, H.(*) &
Nat. Mater. 2023, 22, 18-35. DOI: 10.1038/s41563-022-01384-1. (IF 46)

124. "Adsorption and Diffusion of Oxygen on Pure and Partially Oxidized Metal Surfaces in Ultrahigh Resolution"
Kanhaiya, K. (GS); Heinz, H. (*) &
Nano Lett. 2022, 22, 5392-5400. DOI: 10.1021/acs.nanolett.2c00490 (IF 11)

123. "Patterning of Self-Assembled Monolayers of Amphiphilic Multisegment Ligands on Nanoparticles and Design Parameters for Protein Interactions"
Hoff, S. E. (GS); Di Silvio, D.; Moya, S. E.; Ziolo, R. F.; **Heinz, H.** (*) &

ACS Nano 2022, 16, 8766-8783. DOI: 10.1021/acsnano.1c08695 (IF 16)

122. „Amelogenin Nanoribbon Secondary Structure Provides a Low-Energy Template for Mineral Nucleation“
Akkineni, S.; Zhu, C. (PD); Chen, J.; Song, M.; Hoff, S. E. (GS); Bonde, J.; Tao, J.; **Heinz, H. (*)**; Habelitz, S. (*); De Yoreo, J. J. (*) &
Proc. Natl. Acad. Sci. USA 2022, 119, e2106965119. DOI: 10.1073/pnas.210696511 (IF 11)

121. „Binding of Polar and Hydrophobic Molecules at the LiCoO2 (001)-Water Interface: Force Field Development and Molecular Dynamics Simulations “
Liang, D.; Liu, J. (PD); Heinz, H.; Mason, S. E.; Hamers, R. J.; Cui, Q. (*)
Nanoscale 2022, 14, 7003-7014. DOI: 10.1039/d2nr00672c (IF 7.8)

120. “Molecular Modeling of Chemical Admixtures; Opportunities and Challenges”
Mohamed, A. K.; Weckwerth, S. A.; Mishra, R. K.; Heinz, H.; Flatt, R. J.
Cem. Concr. Res. 2022, 156, 106783. DOI: 10.1016/j.cemconres.2022.106783 (IF 10.5)

119.* “Surface Patterning in Alloys”
Heinz, H. (*)
Nat. Synth. 2022, 1, 103-104. DOI: 10.1038/s44160-022-00028-1 (IF expected ~15-20).

118. “CHARMM-GUI Nanomaterial Modeler for Modeling and Simulation of Nanomaterial Systems”
Choi, Y. K.; Kern, N. R.; Kim, S.; Kanhaiya, K. (GS); Afshar, Y.; Jeon, S. H.; Jo, S.; Brooks, B. R.; Lee, J.; Tadmor, E. B.; **Heinz, H.**; Im, W. &
J. Chem. Theor. Comput. 2022, 18, 479-493. DOI: 10.1021/acs.jctc.1c00996 (IF 6.0)

117. “Binding Mechanism and Binding Free Energy of Amino Acids and Citrate to Hydroxyapatite Surfaces as a Function of Crystallographic Facet, pH, and Electrolytes”
Hoff, S. E. (GS); Liu, J. (PD); **Heinz, H.** (*) &
J. Colloid Interface Sci. 2022, 605, 685-700. DOI: 10.1016/j.jcis.2021.07.109. (IF 8.1)

116. “Prediction of Carbon Nanotube and Carbon Fiber Mechanical Properties Using Reactive Simulations and Machine Learning”
Zhao, Q.; Winetrout, J. J. (GS); Xu, Y.; Wang, Y. (*); **Heinz, H.** (*) &
arXiv preprint 2021, arXiv:2110.00517.

115. “Molecular Dynamics Modeling of Epoxy Resins using the Reactive Interface Force Field”
Odegard, G. M. (*); Pail, S. U.; Deshpande, P.; Kanhaiya, K. (GS); Winetrout, J. J. (GS); **Heinz, H.**; Shah, S.; Maiaru, M. &
Macromolecules 2021, 54, 9815-9824. DOI: 10.1021/acs.macromol.1c01813 (IF 6.0)

114. “Anchoring of a Hydrophobic Heptapeptide (AFILPTG) on Silica Facilitates Peptide Unfolding at the Abiotic–Biotic Interface”
Volkov, V. V.; **Heinz, H.**; Perry, C. C.
Phys. Chem. Chem. Phys. 2021, 23, 18001-18011. DOI: 10.1039/D1CP02072B. (IF 3.7)

113.* "Simulations of Clay Minerals with IFF All Atom Models: Concepts, Validation, and Applications"
Jamil, T. (GS); **Heinz, H. (*)** &
In "Computational Modeling in Clay Mineralogy", Sainz-Diaz, I., Ed.; Volume 3, Pages 54-73. AIPEA Educational Series, Publication No. 3, Pages 54-73. Digilabs, Bari, Italy, 2021. DOI: 10.14644/AES.003. ISBN: 978-88-7522-048-8.

112. "Accurate and Compatible Force Fields for Molecular Oxygen, Nitrogen, and Hydrogen to Simulate Gases, Electrolytes, and Heterogeneous Interfaces"
Wang, S. (GS); Hou, K. (UGS); **Heinz, H.** (*) &
J. Chem. Theor. Comput. 2021, 17, 5198-5213. DOI: 10.1021/acs.jctc.0c01132 (IF 5.3)

111. "Direct Correlation of Oxygen Adsorption on Platinum Electrolyte Interfaces with the Activity in the Oxygen Reduction Reaction"
Wang, S. (GS); Zhu, E.; Huang, Y.; **Heinz, H.** (*) &
Sci. Adv. 2021, 7, eabb1435. DOI: 10.1126/sciadv.abb1435 (IF 13)

110. "Working Mechanisms and Design Principles of Comb-like Polycarboxylate Ether Superplasticizers in Cement Hydration: Quantitative Insights for a Series of Well-Defined Copolymers"
Javadi, A. (GS); Jamil, T. (GS); Abouzari-Lotf, E.; Soucek, M. D. (*); **Heinz, H.** (*) &
ACS Sustainable Chem. Eng. 2021, 9, 8354-8371. DOI: 10.1021/acssuschemeng.0c08566 (IF 7.6) (Cover Art, June 28, https://pubs.acs.org/toc/ascecg/9/25)

109.* "Cement Interfaces: Current Understanding, Challenges, and Opportunities"
Heinz, O.; **Heinz. H. (*)**
Langmuir 2021, 37, 6347-6356. DOI: 10.1021/acs.langmuir.1c00617 (IF 3.5)

108.* "Multiscale Experiments and Modeling in Biomaterials and Biological Materials, Part I"
Du, J.; Katti, D.; **Heinz, H.**
JOM 2021, 73, 1673-1675. DOI: 10.1007/s11837-021-04692-0 (IF 2.3)

107. "Accurate Simulation of Surfaces and Interfaces of Ten Face-Centered Cubic Metals and Steel Using Lennard-Jones Potentials"
Kanhaiya, K. (GS); Kim, S.; Im, W.; **Heinz, H.** (*) &
NPJ Comput. Mater. 2021, 7, 1-15. DOI: 10.1038/s41524-020-00478-1. (IF 9.3)

106. "Force Field for Calcium Sulfate Minerals to Predict Structural, Hydration, and Interfacial Properties"
Mishra, R. K. (GS); Kanhaiya, K. (GS); Winetrout, J. (GS); Flatt, R. J.; **Heinz, H.** (*) &
Cem. Concr. Res. 2021, 139, 106262. DOI: 10.1016/j.cemconres.2020.106262 (IF 8.3)

105. "Involvement of Prenucleation Clusters in Calcium Phosphate Mineralization of Collagen"
Ma, Y.-X.; Hoff, S. E. (GS); Huang, X.-Q.; Liu, J.; Wan, Q.-Q.; Song, Q.; Gu, J-T.; **Heinz, H.** (*); Tay, F. R. (*); Niu, L.-N. (*) &
Acta Biomater. 2021, 120, 213-223. DOI: 10.1016/j.actbio.2020.07.038. (IF 7.2)

104. "Interaction of Poly(methyl acrylate) with Carbon Nanotubes as a Function of CNT

Diameter, Chirality, and Temperature"
Garley, A. (GS); Arias-Monje P. J.; Hoff, S. E. (GS); Sharp, M. (UGS); Kumar, S.; **Heinz, H.** (*) &
J. Phys. Chem. C 2020, 124, 25632-25644. DOI: 10.1021/acs.jpcc.0c08626 (IF 4.1)

103. "Post-Synthetic Modification of Ionic Liquids Using Ligand-Exchange and Redox Coordination Chemistry"
LeRoy, M.; Mroz, A. M.; Mancuso, J. L.; Miller, A.; Van Cleve, A.; Check, C.; **Heinz, H.**; Hendon, C. A.; Brozek, C. K. (*)
J. Mater. Chem. A 2020, 8, 22674-22685. DOI: 10.1039/D0TA06195F (IF 11.3)

102. "ReaxFF Reactive Force Field Study of Polymerization of Polymer Matrix in Carbon Nanotube – Composite System"
Damirchi, B.; Radue, M; Kanhaiya, K. (GS); **Heinz, H.**; Odegard, G.; Van Duin, A. C. T. (*) &
J. Phys. Chem. C 2020, 124, 20488-20497. DOI: 10.1021/acs.jpcc.0c03509 (IF 4.1)

101. "Molecular Dynamics Simulations of Separator-Cathode Interfacial Thermal Transport in a Li-ion Cell"
Dhakane, A.; Varshney, V.; Liu, J. (PD); **Heinz, H.**; Jain, A. (*)
Surfaces and Interfaces 2020, 100674. DOI: 10.1016/j.surfin.2020.100674 (IF 3.7)

100. "Enhancement of Oxygen Reduction Reaction Activity by Grain Boundaries in Platinum Nanostructure"
Zhu, E.; Xue, W.; Wang, S. (GS); Yan, X.; Zhou, J.; Liu, Y.; Cai, J.; Liu, E.; Jia, Q.; Duan, X.; Li, Y.; **Heinz, H.** (*); Huang, Y. (*) &
Nano Res. 2020, 13, 3310-3314. DOI: 10.1007/s12274-020-3007-2. (IF 8.2)

99. "Interpretable Molecular Models for Molybdenum Disulfide and Insight into Selective Peptide Recognition"
Liu, J. (PD); Zeng, J. (UGS); Zhu, C. (PD); Miao, J.; Huang, Y.; **Heinz, H.** (*) &
Chem. Sci. 2020, 11, 8708-8722. DOI: 10.1039/D0SC01443E. (IF 9.3)
(Cover Art, Sep 7:
https://pubs.rsc.org/en/content/articlepdf/2020/sc/d0sc90185g?page=search)

98. "Understanding Surface Reactivity of Ligand-Protected Metal Nanoparticles for Biomass Upgrading"
Mark, L. O. (GS); Zhu, C. (PD); Medlin, J. W.; **Heinz, H.** (*) &
ACS Catal. 2020, 10, 5462-5474. DOI: 10.1021/acscatal.9b04772 (IF 12)
(Cover Art, May 15: https://pubs.acs.org/toc/accacs/10/10)

97. "Vaporizable Endoskeletal Droplets via Tunable Interfacial Melting Transitions"
Shakya, G.; Hoff, S. E. (GS); Wang, S. (GS); **Heinz, H.**; Ding, X; Borden, M. (*) &
Sci. Adv. 2020, 6, eaaz7188. DOI: 10.1126/sciadv.aaz7188 (IF 12)

96. "Reactive Modeling of Mo3Si Oxidation and Resulting Silica Morphology"
Dharmawardhana, C. C. (PD); Zhou, J.; Taylor, M.; Miao, J.; Perepezko, J. H.; **Heinz, H.** (*) &

Acta Mater. 2020, 187, 93-102. DOI: 10.1016/j.actamat.2020.01.048 (IF 7.3)

95. "Mechanism of Molecular Interaction of Acrylate-Polyethylene Glycol Acrylate Copolymers with Calcium Silicate Hydrate Surfaces"
Jamil, T. (GS); Javadi, A. (GS); **Heinz, H.** (*) &
Green Chem. 2020, 22, 1577-1593. DOI: 10.1039/C9GC03287H (IF 9.4)
(Cover Art, Mar 7:
https://pubs.rsc.org/en/content/articlelanding/2020/gc/d0gc90026e/unauth#!divAbstract)

94. "Polyacrylonitrile Interactions with Carbon Nanotubes in Solution: Conformations and Binding as a Function of Solvent, Temperature, and Concentration"
Pramanik, C. (PD); Jamil, T. (GS); Gissinger, J. R. (GS); Guittet, D. (UGS); Arias-Monje, P. J.; Kumar, S.; **Heinz, H.** (*) &
Adv. Funct. Mater. 2019, 29, 1905247. DOI: 10.1002/adfm.201905247 (IF 16)

93. "Single- and Multi-Component Chiral Supraparticles as Modular Enantioselective Catalysts"
Li, S.; Liu, J. (PD); Ramesar, N.; Xu, L.; **Heinz, H.**; Xu, C. (*); Kotov, N. (*) &
Nat. Comm. 2019, 10, 4826. DOI: 10.1038/s41467-019-12134-4 (IF 12)

92. "Peptide-Assisted 2-D Assembly toward Free-Floating Ultrathin Platinum Nanoplates as Effective Electrocatalysts"
Zhu, E.; Yan, X.; Wang, S. (GS); Xu, M.; Wang, C.; Liu, H.; Huang, J.; Xue, W.; Cai, J.; **Heinz, H.**; Li, Y.; Huang, Y. (*) &
Nano Lett. 2019, 19, 3730-3736. DOI:
https://pubs.acs.org/doi/10.1021/acs.nanolett.9b00867 (IF 12)

91. "Constructing Realistic Surface Models of Silicate Glasses using Molecular Dynamics to Understand the Effect of pH on the Hydration Properties"
Stewart, R. (*); Goyal, S.; Lee, S. H.; Rammohan, A.; Park, H. H.; Min, K.; Cho, E.; **Heinz, H.**
J. Chem. Phys. 2019, 150, 174703. DOI: 10.1063/1.5084334 (IF 3.0)

90. "Dynamics of Carbohydrate Strands in Water and Interactions with Clay Minerals: Influence of pH, Surface Chemistry, and Electrolytes"
Jamil, T. (GS); Garley, A. (GS); Gissinger, J. (GS); Saikia, N. (PD); Upadhyay, A.; **Heinz, H.** (*) &
Nanoscale 2019, 11, 11183-11194. DOI: 10.1039/c9nr01867k (IF 7.0)

89. "Adsorption and Substitution of Metal Ions on Hydroxyapatite as a Function of Crystal Facet and Electrolyte pH"
Garley, A. (GS); Hoff, S. E. (GS); Saikia, N. (PD); Jamadagni, S.; Baig, A.; **Heinz, H.** (*) &
J. Phys. Chem. C 2019, 123, 16982-16993. DOI: 10.1021/acs.jpcc.9b02808 (IF 4.3)
(Cover Art, July 11, https://pubs.acs.org/toc/jpccck/123/27)

88. "Observing Crystal Nucleation in Four Dimensions using Atomic Electron Tomography"
Zhou, J.; Yang, Y.; Yang, Y.; Kim, D. S.; Yuan, A.; Tian, X.; Ophus, C.; Sun, F.; Schmid,

A. K.; Nathanson, M. (GS); **Heinz, H.**; An, Q.; Zeng, H.; Ercius, P.; Miao, J. (*) &
Nature 2019, 570, 500-503. DOI: doi:10.1038/s41586-019-1317-x (IF 43)

87. "From Phage Display to Structure: Interplay of Enthalpy and Entropy in Binding of LDHSLHS Polypeptide to Silica"
Oliver, D.; Michaelis, M.; **Heinz, H.**; Volkov, V. V.; Perry, C. C. (*)
Phys. Chem. Chem. Phys. 2019, 21, 4663-4672. DOI: 10.1039/C8CP07011C (IF 3.6)

86. "Long-Range Hierarchical Nanocrystal Assembly Driven by Molecular Structural Transformation"
Zhu, E.; Wang, S. (GS); Yan, X.; Sobani, M. (GS); Ruan, L.; Wang, C.; Liu, Y.; Duan, X.; **Heinz, H.** (*); Huang, Y. (*) &
J. Am. Chem. Soc. 2019, 141, 1498-1505. DOI: 10.1021/jacs.8b08023 (IF 14)
(Cover Art, Jan 30, https://pubs.acs.org/toc/jacsat/141/4)

85. "Atomic-Scale Structure and Stress Release Mechanism in Core-Shell Nanoparticles"
Nathanson, M. (GS); Kanhaiya, K. (GS); Pryor, Jr., A.; Miao, J.; **Heinz, H.** (*) &
ACS Nano 2018, 12, 12296-12304. DOI: 10.1021/acsnano.8b06118 (IF 14)

84. "Building Two-Dimensional Materials One Row at a Time: Avoiding the Nucleation Barrier"
Chen, J.; Zhu, E.; Liu, J. (PD); Zhang, S.; Lin, Z.; Duan, X.; **Heinz, H.**; Huang, Y. (*); De Yoreo, J. J. (*) &
Science 2018, 362, 1135-1139. DOI: 10.1126/science.aau4146 (IF 41)

83. "Furfuryl Alcohol Deoxygenation, Decarbonylation, and Ring-Opening on Pt(111)"
Mark, L. O. (GS); Jenkins, A. H.; **Heinz, H.**; Medlin, J. W. (*) &
Surf. Sci. 2018, 677, 333-340. DOI: 10.1016/j.susc.2018.07.001 (IF 2.0)

82. "Interactions at the Silica-Peptide Interface: Influence of the Extent of Functionalization on the Conformational Ensemble"
Sola-Rabada, A.; Michaelis, M.; Roe, M.; Oliver, D. J.; Colombi Ciacchi, L.; **Heinz, H.**; Perry, C. C. (*)
Langmuir 2018, 34, 8255-8263. DOI: 10.1021/acs.langmuir.8b00874 (IF 3.8)

81. "Understanding Chemical Bonding in Alloys and the Representation in Atomistic Simulations"
Liu, J. (PD); Tennessen, E.; Miao, J.; Huang, Y.; Rondinelli, J. M.; **Heinz, H.** (*) &
J. Phys. Chem. C 2018, 122, 14996-15009. DOI: 10.1021/acs.jpcc.8b01891 (IF 4.5)

80. "Single-Shot 3D Coherent Diffractive Imaging of Core-Shell Nanoparticles with Elemental Specificity"
Pryor, A., Jr.; Rana, A.; Xu, R.; Rodriguez, J. A.; Yang, Y.; Gallagher-Jones, M.; Jiang, H.; Kanhaiya, K. (GS); Nathanson, M. (GS); Park, J.; Kim, Sunam; Kim, Sangsoo; Nam, D.; Yue, Y.; Fan, J.; Sun, Z.; Zhang, B.; Gardner, D. F.; Baraldi Dias, C. S.; Joti, Y.; Hatsui, T.; Kameshima, T.; Inubushi, Y.; Tono, K.; Lee, J. Y.; Yabashi, M.; Song, C.; Ishikawa, T.; Kapteyn, H. C.; Murnane, M. M.; **Heinz, H.**; Miao, J. (*) &
Sci. Rep. 2018, 8, 8284. DOI: 10.1038/s41598-018-26182-1 (IF 4.1)

79. “Quantitative Characterization of High Temperature Oxidation Using Electron Tomography and Energy-Dispersive X-ray Spectroscopy“
Zhou, J.; Taylor, M.; Melinte, G. A.; Shahani, A. J.; Dharmawardhana, C. C. (PD); **Heinz, H.**; Voorhees, P. W.; Perepezko, J. H.; Bustillo, K.; Ercius, P.; Miao, J. (*) &
Sci. Rep. 2018, 8, 10239. DOI: 10.1038/s41598-018-28348-3 (IF 4.1)

78. „Molecular Structure and Assembly of Peptide-Derived Nanomaterials“
Liu, J. (PD); Wang, Z. (UGS); Zeng, J. (UGS); **Heinz, H.** (*) &
Curr. Opin. Green Sust. Chem. 2018, 12, 38-46. DOI: 10.1016/j.cogsc.2018.05.007 (IF ~5)

77. „Molecular Engineering of Interphases in Polymer/Carbon Nanotube Composites to Reach the Limits of Mechanical Performance“
Pramanik, C. (PD); Nepal, D.; Nathanson, M. (GS); Gissinger, J. R. (GS); Garley, A. (GS); Berry, R. J.; Davijani, A.; Kumar, S.; **Heinz, H.** (*) &
Compos. Sci. Tech. 2018, 29, 86-94. DOI: 10.1016/j.compscitech.2018.04.013 (IF 5.2)

76. “Nanoscale Structure-Property Relationships of Polyacrylonitrile/CNT Composites as a Function of Polymer Crystallinity and CNT Diameter”
Gissinger, J. R. (GS); Pramanik, C. (PD); Newcomb, B.; Kumar, S.; **Heinz, H.** (*) &
ACS Appl. Mater. Interfaces 2018, 10, 1017-1027. DOI: 10.1021/acsami.1027b09739 (IF 7.5)

75. “Instantaneous Insight into Induced Charges at Metal Surfaces, Aqueous, and Biological Interfaces Using a Polarizable Lennard-Jones Potential”
Lorenzo Geada, I. (GS in Germany co-advised with Sulpizi); Ramezani-Dakhel, H. (GS); Jamil, T. (GS), Sulpizi, M. (*); **Heinz, H.** (*) &
Nat. Comm. 2018, 9, 716. DOI: 10.1038/s41467-018-03137-8 (IF 12)

74. “Carbon Nanotube Dispersion in Solvents and Polymer Solutions: Mechanisms, Assembly, and Preferences”
Pramanik, C. (PD); Gissinger, J. R. (GS); Kumar, S.; **Heinz, H.** (*) &
ACS Nano 2017, 11, 12805-12816. DOI: 10.1021/acsnano.7b07684 (IF 13)

73. “CEMFF: A Force Field Database for Cementitious Materials Including Validations, Applications and Opportunities”
Mishra, R. K. (GS) (*); Mohamed, A. K.; Geissbuhler, D.; Manzano, H.; Jamil, T.; Shahsavari, R. (*); Kalinichev, A. G.; Galmarini, S.; Tao, L.; **Heinz, H.**; Pellenq, R.; van Duin, A. C. T.; Parker, S. C.; Flatt, R.; Bowen, P. (*) &
Cem. Conr. Res. 2017, 102, 68-89. DOI: 10.1016/j.cemconres.2017.09.003 (IF 7.8)

72.* “Energy-effective Grinding of Inorganic Solids Using Organic Additives“
Mishra, R. K. (GS); Weibel, M.; Muller, T.; **Heinz, H.**; Flatt, R. J. (*) &
Chimia 2017, 71, 451-460. DOI: 10.2533/chimia.2017.451. 2016 Sandmeyer Award Lecture (Swiss Chemical Society). (IF 1.0)

71.* “Reliable Computational Design of Biological-Inorganic Materials to the Large Nanometer Scale Using Interface-FF”

Dharmawardhana, C. C. (PD); Kanhaiya, K. (GS); Lin, T.-J. (GS); Garley, A. (GS); Knecht, M. R.; Zhou, J.; Miao, J.; **Heinz, H.** (*) &
Mol. Sim. 2017, 43, 1394-1405. DOI: 10.1080/08927022.2017.1332414 (IF 1.0)

70. "Influence of Aluminates on the Hydration Kinetics of Tricalcium Silicate"
Pustovgar, E.; Mishra, R. K. (GS); Palacios, M.; d'Espinose de Lacaillerie, J. B.; Matschei, T.; Andreev, A.; **Heinz, H.**; Verel, R.; Flatt, R. J. (*) &
Cem. Concr. Res. 2017, 100, 245-262. DOI: 10.1016/j.cemconres.2017.06.006 (IF 4.8)

69. "Nature of Peptide Wrapping onto Metal Nanoparticle Catalysts and Driving Forces for Size Control"
Ramezani-Dakhel, H. (GS); Bedford, N. M; Woehl, T. J.; Knecht, M. R.; Naik, R. R.; **Heinz, H.** (*) &
Nanoscale 2017, 9, 8401-8409. DOI: 10.1039/C7NR02813J (IF 7.8)

68.* "Nanoparticle Decoration with Surfactants: Molecular Interactions, Assembly, and Applications"
Heinz, H. (*); Pramanik, C. (PD); Heinz, O.; Ding, Y.; Mishra, R. K. (GS); Marchon, D.; Flatt, R. J.; Estrela-Lopis, I.; Llop, J.; Moya, S.; Ziolo, R. F. &
Surf. Sci. Rep. 2017, 72, 1-58. DOI: 10.1016/j.surfrep.2017.02.001 (IF 17)

67. "A Study of the Impact of Polyanions on the Formation of Lipid Bilayers on Top of Polyelectrolyte Multilayers with Poly(allylamine hydrochloride) as Top Layer"
Diamanti, E.; Andreozzi, P.; Kirby, C. (UGS); Anguiano, R.; Yate, L.; **Heinz, H.**; Ziolo, R.; Donath, E.; Moya, S. (*) &
J. Phys. Chem. B 2017, 121, 1158-1167. DOI: 10.1021/acs.jpcb.6b12237 (IF 3.2)

66. "Accurate Force Field Parameters and pH Resolved Surface Models for Hydroxyapatite to Understand Structure, Mechanics, Hydration, and Biological Interfaces"
Lin, T. Z. (GS); **Heinz, H.** (*) &
J. Phys. Chem. C 2016, 120, 4975-4992. DOI: 10.1021/acs.jpcc.5b12504 (IF 4.1)

65. "Correction to Force Field and a Surface Model Database for Silica to Simulate Interfacial Properties in Atomic Resolution"
Emami, F. S. (GS); Puddu, V.; Berry, R. J.; Varshney, V.; Patwardhan, S. V.; Perry, C. C.; **Heinz, H.** (*) &
Chem. Mater. 2016, 28, 406-407. DOI: 10.1021/acs.chemmater.5b04760 (IF 10)

64.* "Adsorption of Biomolecules and Polymers on Silicates, Glasses, and Oxides: Mechanisms, Predictions, and Opportunities by Molecular Simulation"
Heinz, H. (*)
Curr. Op. Chem. Eng. 2016, 11, 34-41. DOI: 10.1016/j.coche.2015.12.003 (IF 5.1)

63.* "Simulations of Inorganic-Bioorganic Interfaces and Comparisons to Experiment to Discover New Materials: Progress, Challenges, and Opportunities"
Heinz, H. (*); Ramezani-Dakhel, H. (GS) &
Chem. Soc. Rev. 2016, 45, 412-448. DOI: 10.1039/C5CS00890E (IF 40)

62. ”Three-Dimensional Positions of Individual Atoms in Materials Revealed by Electron Tomography”
Xu, R.; Chen, C. C.; Wu, L.; Scott, M. C.; Theis, W.; Ophus, C.; Bartels, M.; Yang, Y.; Ramezani-Dakhel (GS), H.; Sawaya, M. R.; **Heinz, H.**; Marks, L. D.; Ercius, P.; Miao, J. (*) &
Nat. Mater. 2015, 14, 1099-1103. DOI: 10.1038/nmat4426 (IF 40)

61. “Atomic-Scale Identification of Pd Leaching in Nanoparticle Catalyzed CC Coupling: Effects of Particle Surface Disorder”
Briggs, B.; Bedford, N.; Seifert, S.; Koerner, H.; Ramezani-Dakhel, H. (GS); **Heinz, H.**; Naik, R. R.; Frenkel, A.; Knecht, M. R. (*) &
Chem. Sci. 2015, 6, 6413-6419. DOI: 10.1039/C5SC01424G (IF 9.1)

60. “En Route to a Multi-Model Scheme for Clinker Comminution with Chemical Grinding Aids”
Mishra, R. K. (GS); Geissbuehler, D.; Carmona, H.; Wittel, F. K.; Sawley, M. L.; Weibel, M.; Gallucci, E.; Herrmann, H. J.; **Heinz, H.**; Flatt, R. J. (*) &
Adv. Appl. Ceram. 2015, 114, 393-401. DOI: 10.1179/1743676115Y.0000000023 (IF 1.1)

59. “Elucidation of Peptide-Directed Palladium Surface Structure for Biologically-Tunable Nanocatalysts”
Bedford, N. M.; Ramezani-Dakhel, H. (GS); Slocik, J. M.; Briggs, B. D.; Ren, Y.; Frenkel, A. I.; Petkov, V.; **Heinz, H.**; Naik, R. R.; Knecht, M. R. (*) &
ACS Nano 2015, 9, 5082-5092. DOI: 10.1021/acsnano.5b00168. Cover Art (May). (IF 13)

58. “Molecular Mechanism of Specific Recognition of Cubic Pt Nanocrystals by Peptides and of the Concentration-Dependent Formation from Seed Crystals”
Ramezani-Dakhel, H. (GS); Ruan, L.; Huang, Y. (*); **Heinz, H.** (*) &
Adv. Funct. Mater. 2015, 25, 1374-1384. DOI: 10.1002/adfm.201404136 (IF 15)

57. “Prediction of Specific Biomolecule Adsorption on Silica Surfaces as a Function of pH and Particle Size”
Emami, F. S. (GS); Puddu, V.; Berry, R. J.; Varshney, V.; Patwardhan, S. V.; Perry, C. C.(*); **Heinz, H.** (*) &
Chem. Mater. 2014, 26, 5725-5734. DOI: 10.1021/cm5026987 (IF 10)

56. “A Rational Biomimetic Approach to Structure Defect Generation in Colloidal Nanocrystals”
Ruan, L.; Ramezani-Dakhel, H. (GS); Lee, C.; Li, Y.; Duan, X.; **Heinz, H.**; Huang, Y. (*) &
ACS Nano 2014, 8, 6934-6944. DOI: 10.1021/nn501704k (IF 13)

55.* “The Role of Chemistry and pH of Solid Surfaces for Specific Adsorption of Biomolecules in Solution—Accurate Computational Models and Experiment”
Heinz, H. (*)
J. Phys.: Condens. Matter 2014, 26, 244105. DOI: 10.1088/0953-8984/26/24/244105 (IF 2.6)

54.* "A Force Field for Tricalcium Aluminate to Characterize Surface Properties, Initial Hydration, and Organically Modified Interfaces in Atomic Resolution"
Mishra, R. K. (GS); Fernandez-Carrasco, L.; Flatt, R. J.; **Heinz, H.** (*) &
Dalton Trans. 2014, 43, 10602-10616. DOI: 10.1039/C4DT00438H (IF 4.1)

53. "Interaction of Substituted Poly(phenyleneethynylene)s with Ligand-Stabilized CdS Nanoparticles"
Liu, H. (GS); Espe, M. P.; Modarelli, D. A.; Arias, E.; Moggio, I.; Ziolo, R. F.; **Heinz, H.** (*) &
J. Mater. Chem. A 2014, 2, 8705-8711. DOI: 10.1039/C4TA01280A (IF 11.3)

52.* "Understanding Molecular Recognition on Metallic and Oxidic Nanostructures from a Perspective of Computer Simulation and Theory"
Heinz, H. (*)
In "Bio-Inspired Nanotechnology"; Knecht, M. R., Walsh, T. R., Eds.; Springer, New York, 2014, p. 141-171. DOI: 10.1007/978-1-4614-9446-1_6.

51. "Force Field and a Surface Model Database for Silica to Simulate Interfacial Properties in Atomic Resolution"(*)
Emami, F. S. (GS); Puddu, V.; Berry, R. J.; Varshney, V.; Patwardhan, S. V.; Perry, C. C.; **Heinz, H.** (*) &
Chem. Mater. 2014, 26, 2647-2658. DOI: 10.1021/cm500365c (IF 10)

50. "Facet Recognition and Molecular Ordering of Ionic Liquids on Metal Surfaces"
Jha, K. C. (GS); Liu, H. (GS); Bockstaller, M. R.; **Heinz, H.** (*) &
J. Phys. Chem. C 2013, 117, 25969-25981. DOI: 10.1021/jp4032404 (IF 4.1)

49. "Exploiting Localized Surface Binding Effects to Enhance the Catalytic Reactivity of Peptide-Capped Nanoparticles"
Coppage, R.; Slocik, J. M.; Ramezani-Dakhel, H. (GS); Bedford, N. M.; **Heinz, H.**; Naik, R. R.; Knecht, M. R. (*) &
J. Am. Chem. Soc. 2013, 135, 11048-11054. DOI: 10.1021/ja402215t (IF 14)

48. "Force Field for Tricalcium Silicate and Insight into Nanoscale Properties: Cleavage, Initial Hydration, and Adsorption of Organic Molecules"
Mishra, R. K. (GS); Flatt. R. J.; **Heinz, H.** (*) &
J. Phys. Chem. C 2013, 117, 10417-10432. Journal Cover (May 23).
DOI: 10.1021/jp312815g (IF 4.1)

47. "Stability, Surface Features, and Atom Leaching of Palladium Nanoparticles: Toward Prediction of Catalytic Functionality"
Ramezani-Dakhel, H. (GS); Mirau, P. A.; Naik, R. R.; Knecht, M. R.; **Heinz, H.** (*) &
Phys. Chem. Chem. Phys. 2013, 15, 5488-5492. DOI: 10.1039/C3CP00135K (IF 3.9)

46. "Tailoring Molecular Specificity toward a Crystals Facet: A Lesson from Biorecognition Toward Pt{111}"
Ruan, L. Y.; Ramezani-Dakhel, H. (GS); Chiu, C. Y.; Zhu, E. B.; Li, Y. J.; **Heinz, H.** (*); Huang, Y. (*) &

Nano Lett. 2013, 13, 840-846. DOI: 10.1021/nl400022g (IF 12)

45.* "Thermodynamically Consistent Force Fields and Molecular Models for the Assembly of Inorganic, Organic, and Biological Hybrid Nanostructures: The INTERFACE Force Field"
Heinz, H. (*); Lin, T. Z. (GS); Mishra, R. K. (GS); Emami, F. S. (GS) &
Langmuir 2013, 29, 1754-1765. Invited Feature Article and Cover Art (Feb 12).
DOI: 10.1021/la3038846 (IF 3.8)

44. "Understanding the Effectiveness of Polycarboxylates as Grinding Aids"
Mishra, R. K. (GS); **Heinz, H.**; Müller, T.; Zimmermann, J.; Flatt, R. J. (*) &
American Concrete Institute Symposium Series, Vol. 288, Malhotra, V., ed., 2012. Article No 288.16, p. 235-251. ISBN 9781622766406. PDF

43.* "Clay Minerals for Nanocomposites and Biotechnology: Surface Modification, Dynamics, and Responses to Stimuli"
Heinz, H. (*)
Clay Miner. 2012, 47, 205-230. Invited script of George Brown Lecture.
DOI: 10.1180/claymin.2012.047.2.05 (IF 1.0)

42. "Chemistry of Aqueous Silica Nanoparticle Surfaces and the Mechanism of Selective Peptide Adsorption"
Patwardhan, S. V.; Emami, F. S. (GS); Berry, R. J.; Jones, S. E.; Naik, R. R.; Deschaume, O.; **Heinz, H.** (*); Perry, C. C. (*) &
J. Am. Chem. Soc. 2012, 134, 6244-6256. DOI: 10.1021/ja211307u (IF 15)

41. "Influence of the Shape of Nanostructured Metal Surfaces on Adsorption of Single Peptides in Aqueous Solution"
Feng, J. (PD); Slocik, J. M.; Sarikaya, M.; Naik, R. R.; Farmer, B. L.; **Heinz, H.** (*) &
Small 2012, 8, 1049-1059. DOI: 10.1002/smll.201102066 (IF 11.5)

40.* "Alkylammonium Chains on Layered Silicate Surfaces"
Heinz, H. (*)
In "Rubber-Clay Nanocomposites: Science, Technology and Applications"; Galimberti, M., ed.; Wiley and Sons: Hoboken, NJ, 2011, p. 101-126. ISBN 978-0-470-56210-9.

39. "Control over Self-Assembly of Diblock Copolymers on Hexagonal and Square Templates for High Area Density Circuit Boards"
Feng, J. (PD); Cavicchi, K. A.; **Heinz, H.** (*) &
ACS Nano 2011, 5, 9413-9420. DOI: 10.1021/nn2035439 (IF 13)

38. "Bending of Layered Silicates on the Nanometer Scale: Mechanism, Stored Energy, and Curvature Limits"
Fu, Y. T. (GS); Zartman, G. D. (UGS); Yoonessi, M.; Drummy, L. F.; **Heinz, H.** (*) &
J. Phys. Chem. C 2011, 115, 22292-22300. DOI: 10.1021/jp208383f (IF 4.1)

37. "Morphology of Sulfonated Polyarylenethioethersulfone Random Copolymer Series as Proton Exchange Fuel Cells Membranes by Small Angle Neutron Scattering"
Yoonessi, M.; **Heinz, H.**; Bai, Z. W.; Dang, T. D. (*)

Polymer 2011, 5615-5621. DOI: 10.1016/j.polymer.2011.09.047 (IF 4.2)

36. "Crystallographic Recognition Controls Peptide Binding for Bio-Based Nanomaterials"
Coppage, R.; Slocik, J. M.; Briggs, B. D.; Frenkel, A. I.; **Heinz, H.**; Naik, R. R.; Knecht, M. R. (*)
J. Am. Chem. Soc. 2011, 133, 12346-12349. DOI: 10.1021/ja203726n (IF 15)

35. "Adsorption Mechanism of Single Amino Acid and Surfactant Molecules to Au {111} Surfaces in Aqueous Solution: Design Rules for Metal-Binding Molecules"
Feng, J. (PD); Pandey, R. B.; Berry, R. J.; Farmer, B. L.; Naik, R. R.; **Heinz, H.** (*) &
Soft Matter 2011, 7, 2113-2120. Featured as Hot Article. DOI: 10.1039/C0SM01118E (IF 3.7)

34. "Polarization at Metal-Biomolecular Interfaces in Solution"
Heinz, H. (*); Jha, K. C. (GS); Luettmer-Strathmann, J.; Farmer, B. L.; Naik, R. R. &
J. R. Soc. Interface 2011, 8, 220-232. DOI: 10.1098/rsif.2010.0318 (IF 3.7)

33.* "Modification of Inorganic Fillers and Interfacial Properties in Polyolefin Nanocomposites: Theory versus Experiment"
Feng, J. (PD); **Heinz, H.** (*) &
In "Advances in Polyolefin Nanocomposites"; Mittal, V., ed.; CRC Press: Boca Raton, 2010, 205-223. ISBN 978-1-439814543.

32.* "Molecular Simulation of Polymer Melts and Blends: Methods, Phase Behavior, Interfaces, and Surfaces"
Virnau, P.; Binder, K.; **Heinz, H.**; Kreer, T.; Müller, M. (*)
In "Encyclopedia of Polymer Blends"; Isayev, A. I., ed.; Volume 1 "Fundamentals"; Wiley-VCH: Weinheim, 2010, p. 1-44. ISBN: 978-3-527-31928-2.

31.* "Understanding Clay Surface Modification and Organic-Inorganic Interfaces"
Heinz, H. (*)
In "Advances in Polymer Nanocomposite Technology"; Mittal, V., ed.; Nova Science: Hauppauge, NY, 2010, p. 271-291. ISBN 978-1-60741-970-9.

30.* "Simulation of Polymer Matrix Nanocomposites"
Patnaik, S. S; **Heinz, H.**; Pandey, R. B.; Farmer, B. L. (*)
In "Modeling and Simulation in Polymers"; Gujrati, P. D, Leonov, A. I., eds.; Wiley-VCH: Weinheim, 2010, p. 37-92. ISBN: 978-3-527-32415-6.

29. "Layer of Clay Platelets in a Peptide Matrix: Binding, Encapsulation and Morphology"
Pandey, R. B. (*); **Heinz, H.**; Farmer, B. L.; Drummy, L. F.; Jones, S. E.; Vaia, R. A.; Naik, R. R.
J. Polym. Sci. B 2010, 48, 2566-2574. DOI: 10.1002/polb.22140 (IF 2.5)

28. "Bio-functionalization and Immobilization of a Membrane via Peptide Binding (CR31, S2) by a Monte Carlo Simulation"
Pandey, R. B. (*); **Heinz, H.**; Feng, J.; Farmer, B. L.
J. Chem. Phys. 2010, 133, 095102. DOI: 10.1063/1.3484241 (IF 3.0)

27. „Nanostructure and Properties of Sulfonated Polyarylenethioethersulfone Copolymer by Small Angle Neutron Scattering"
Yoonessi, M.; **Heinz, H.**; Dang, T. D.; Wheeler, R.; Bai, Z. W. (*)
Polymer 2010, 51, 1585-1592. DOI: 10.1016/j.polymer.2010.02.011 (IF 4.2)

26. "UV-Absorption and Silica/Titania Colloids Using a Core–Shell Approach"
Zhou, L.; **Heinz, H.**; Soucek, M. D.; Aleman, E. A.; Modarelli, D. A. (*)
Silicon 2010, 2, 95-104. DOI: 10.1007/s12633-009-9030-2 (IF 1.5)

25. "Cleavage Energy of Alkylammonium-Modified Montmorillonite and the Relation to Exfoliation in Nanocomposites: Influence of Cation Density, Head Group Structure, and Chain Length"
Fu, Y. T. (GS); **Heinz, H.** (*) &
Chem. Mater. 2010, 22, 1595-1605. DOI: 10.1021/cm902784r (IF 10)

24.* "Structure and Cleavage Energy of Surfactant-Modified Clay Minerals: Influence of CEC, Head Group, and Chain Length"
Fu, Y. T. (GS); **Heinz, H.** (*) &
Philosophical Magazine 2010, 90, 2415-2424. Invited Paper.
DOI:10.1080/14786430903559490 (IF 1.8)

23. "Nanoscale Tensile, Shear, and Failure Properties of Layered Silicates as a Function of Cation Density and Stress"
Zartman, G. D. (UGS); Liu, H. (GS); Akdim, B.; Pachter, R.; **Heinz, H.** (*) &
J. Phys. Chem. C 2010, 114, 1763-1772. DOI: 10.1021/jp907012w (IF 4.1)

22. "Computational Screening of Biomolecular Adsorption and Self-Assembly on Nanoscale Surfaces"
Heinz, H. (*)
J. Comput. Chem. 2010, 31, 1564-1568. DOI: 10.1002/jcc.21421 (IF 3.2)

21.* "Synthesis, Structure, Characterization, and Properties of Organically Modified Layered Silicates"
Heinz, H. (*)
In "Industry Guide to Polymer Nanocomposites "; Beyer, G., ed.; AMI: Bristol, 2009, p. 7-46. ISBN 978-1-906479046.

20. "Nature of Molecular Interactions of Peptides with Gold, Palladium, and Pd-Au Bimetal Surfaces in Aqueous Solution"
Heinz, H. (*); Farmer, B. L.; Pandey, R. B.; Slocik, J. M.; Patnaik, S. S.; Pachter, R.; Naik, R. R.
J. Am. Chem. Soc. 2009, 131, 9704-9714. DOI: 10.1021/ja900531f (IF 15)

19.* "Molecular Models and Simulations of Layered Materials"
Cygan, R. T. (*); Greathouse, J. A.; **Heinz, H.**; Kalinichev, A. G.
J. Mater. Chem. 2009, 19, 2470-2481. Invited article and journal cover (May 7).
DOI: 10.1039/B819076C (IF 6.6)

18. “Adsorption of peptides (A3, Flg, Pd2, Pd4) on gold and palladium surfaces by a coarse-grained Monte Carlo simulation”
Pandey, R. B. (*); **Heinz, H.**; Feng, J. (PD); Farmer, B. L; Slocik, J. M.; Drummy, L. R.; Naik, R. R.
Phys. Chem. Chem. Phys. 2009, 11, 1989-2001. Invited Paper. DOI: 10.1039/B816187A (IF 3.6)

17. ”Towards Understanding Amino Acid Adsorption at Metallic Interfaces: A Density Functional Theory Study”
Hong, G.; **Heinz, H.**; Naik, R. R.; Farmer, B. L.; Pachter, R. (*)
ACS Appl. Mat. Interf. 2009, 1, 388-392. DOI: 10.1021/am800099z (IF 8.8)

16. “Accurate Simulation of Surfaces and Interfaces of FCC Metals Using 12-6 and 9-6 Lennard-Jones Potentials”
Heinz, H. (*); Vaia, R. A.; Farmer, B. L.; Naik, R. R.
J. Phys. Chem. C 2008, 112, 17281-17290. DOI: 10.1021/jp801931d (IF 4.1)

15. „Photoisomerization of Azobenzene Grafted to Montmorillonite: Simulation and Experimental Challenges”
Heinz, H. (*); Vaia, R. A.; Koerner, H.; Farmer, B. L.
Chem. Mater. 2008, 20, 6444-6456. DOI: 10.1021/cm801287d (IF 10)

14. “Relation between Packing Density and Thermal Transitions of Alkyl Chains on Layered Silicate and Metal Surfaces”
Heinz, H. (*); Vaia, R. A.; Farmer, B. L.
Langmuir 2008, 24, 3727-3733. DOI: 10.1021/la703019e (IF 3.7)

13.* “Calculation of Local and Average Pressure Tensors in Molecular Simulation”
Heinz, H. (*)
Molecular Simulation 2007, 33, 747-758. Invited paper. DOI:10.1080/08927020701308828 (IF 1.7)

12. “Self-Assembly of Alkylammonium Chains on Montmorillonite: Effect of Chain Length, Headgroup Structure, and Cation Exchange Capacity”
Heinz, H. (*); Vaia, R. A.; Krishnamoorti, R.; Farmer, B. L.
Chem. Mater. 2007, 19, 59-68. DOI: 10.1021/cm062019s (IF 10)

11. ”Dynamics of Alkyl Ammonium Intercalants within Organically Modified Montmorillonite: Dielectric Relaxation and Ionic Conductivity”
Jacobs, J. D.; Koerner, H.; **Heinz, H.**; Farmer, B. L.; Mirau, P. A.; Garrett, P. H.; Vaia, R. A. (*)
J. Phys. Chem. B 2006, 110, 20143-20157. DOI: 10.1021/jp061931l (IF 2.9)

10. “Interaction Energy and Surface Reconstruction between Sheets of Layered Silicates“
Heinz, H. (*); Vaia, R. A.; Farmer, B. L.
J. Chem. Phys. 2006, 124, 224713. DOI: 10.1063/1.2202330 (IF 3.0)

9. "Calculation of Local Pressure Tensors in Systems with Many-Body Interactions"
Heinz, H. (*); Paul, W.; Binder, K.
Phys. Rev. E 2005, 72, 066704. DOI: 10.1103/PhysRevE.72.066704 (IF 2.3)

8. „Force Field for Phyllosilicates and Dynamics of Octadecylammonium Chains Grafted to Montmorillonite“
Heinz, H. (*); Koerner, H.; Vaia, R. A.; Anderson, K. L.; Farmer, B. L.
Chem. Mater. 2005, 17, 5658-5669. DOI: 10.1021/cm0509328 (IF 10)

7. "Conformation and Dynamics of a Self-Avoiding Sheet: Bond-Fluctuation Computer Simulation"
Pandey, R. B.; Anderson, K. L.; **Heinz, H.**; Farmer, B. L.
J. Polym. Sci. B 2005, 43, 1041-1046. DOI: 10.1002/polb.20394 (IF 2.5)

6. "Analysis of the Phase Transitions in Alkyl-Mica by Density and Pressure Profiles"
Heinz, H. (*); Paul, W.; Suter, U. W.; Binder, K.
J. Chem. Phys. 2004, 120, 3847-3854. DOI: 10.1063/1.1642605 (IF 3.0)

5. "Surface Structure of Organoclays"
Heinz, H.; Suter, U. W. (*)
Angew. Chem. Int. Ed. 2004, 43, 2239-2243. DOI: 10.1002/anie.200352747 (IF 11)

4. "Atomic Charges for Classical Simulations of Polar Systems"
Heinz, H. (*); Suter, U. W.
J. Phys. Chem. B 2004, 108, 18341-18352. DOI: 10.1021/jp048142t (IF 2.9)

3. "Structure and Phase Transitions of Alkyl Chains on Mica"
Heinz, H.; Castelijns, H. J.; Suter, U. W. (*) &
J. Am. Chem. Soc. 2003, 125, 9500-9510. DOI: 10.1021/ja021248m (IF 15)

2. "Simple and Accurate Computations of Solvatochromic Shifts in pi ->pi* Transitions of Aromatic Chromophores"
Heinz, H.; Suter, U. W.; Leontidis, E. (*)
J. Am. Chem. Soc. 2001, 123, 11229-11236. DOI: 10.1021/ja010396u (IF 15)

1. "Normal and Defective Perylene Substitution Sites in Alkane Crystals"
Leontidis, E.; **Heinz, H.**; Palewska, K.; Wallenborn, E.-U.; Suter, U. W.
J. Chem. Phys. 2001, 114, 3224-3235. DOI: 10.1063/1.1342238 (IF 3.0)

Patents

1. Heinz, H. “Methods and Systems for Accurate Simulation of Surfaces and Interfaces of FCC Metals” PCT Int. Appl. (2009), WO 2009036182 A2 20090319.

Conference Proceedings

(#11, 10, 9, 6, 3, 2, 1 are peer-reviewed)

11. Miao, J. (*); Zhou, J.; Yang, Y.; Yang, Y.; Kim, D. S.; Yuan, A.; Tian, X.; Ophus, C.; Sun, F.; Schmid, A. K.; Nathanson, M.; **Heinz, H.**; An, Q.; Zeng, H.; Ercius, P. &
"4D Atomic Electron Tomography"
Microsc. Microanal. **2019**, 25, 1814-1815. DOI: 10.1017/S1431927619009802

10. Xu, R.; Chen, C. C.; Wu, L.; Scott, M. C.; Theis, W.; Ophus, C.; Bartels, M.; Yang, Y.; Ramezani-Dakhel, H.; Sawaya, M. R.; **Heinz, H.**; Marks, L. D.; Ercius, P.; Miao, J. (*) &
"Three-Dimensional Determination of the Coordinates of Individual Atoms in Materials"
Microsc. Microanal. (Suppl 3) **2016**, 22, 916-917. DOI: 10.1017/S1431927616005420

9. Mishra, R. K.; Flatt, R. J.; **Heinz, H.** (*) &
"Force Field Model of Alite Based on Stoichiometric Analysis"
Proceedings of 35th Cement and Concrete Science Conference **2015**, University of Aberdeen, UK.

8. Mishra, R. K.; Flatt, R. J.; Heinz, H.
"Molecular Understanding of Directional Surface and Interface Tensions of Gypsum and Plaster"
Proc. XIII Int. Congress on the Chemistry of Cement **2011** (Madrid, Spain).

7. Mishra, R. K.; Flatt, R. J.; Heinz, H.
"Cleavage Energy of Tricalcium Silicate and Interactions with Amine Additives"
Proc. XIII Int. Congress on the Chemistry of Cement **2011** (Madrid, Spain).

6. **Heinz, H.**; Drummy, L. R.; Vaia, R. A.; Naik, R. R.; Farmer, B. L.
„Peptide Binding to Sheet Silicate and Metal Nanoparticles: Insight from Atomistic Simulation"
Proc. ACS Div. Polym. Mater. Sci. Eng. **2008**, *98*, 292-295.

5. Heinz, H.; Drummy, L. R.; Vaia, R. A.; Naik, R. R.; Farmer, B. L.
"Modeling Peptides for Binding to Inorganic Surfaces and Thermal Transitions of Alkyl Chains on Flat Surfaces"
Smart Coatings Conference, Orlando, FL; ACS Symp. Ser. **2008**.

4. Heinz, H.; Jha, K. C.; Farmer, B. L.; Naik, R. R.
"Peptide Binding to Sheet Silicate and Metal Nanonoparticles − Insight from Atomistic Simulation"
Proc. SAMPE Fall Technical Conference **2007**.

3. **Heinz, H. (*)**; Vaia, R. A.; Farmer, B. L.
"Free Energy of Exfoliation Between Layered Silicate Sheets"
Proc. ACS Div. Polym. Mater. Sci. Eng. **2005**, *93*, 921-922.

2. **Heinz, H.** (*); Anderson, K. L.; Koerner, H.; Vaia, R. A.; Farmer, B. L.
"Towards Quantitative Modeling of Surface Properties in Inorganic-Organic Hybrid

Materials"
Proc. ACS Div. Polym. Mater. Sci. Eng. **2005**, *93*, 917-918.

1. **Heinz, H.** (*); Vaia, R. A.; Farmer, B. L.
"Self-Assembly of Alkylammonium Chains on Montmorillonite: Effect of Chain Length, Head Group Structure, and Cation Exchange Capacity"
Proc. ACS Div. Polym. Chem. **2005**, *46*, 82-83.

Selected Press and Media Releases

13. 9 News releases related to publication #125 (Hierarchically Structured Bioinspired Nanocomposites), November 2022 to January 2023

12. 10+ News releases related to publication #111 (Correlation of Oxygen Adsorption on Pt with ORR Activity), July 2021

11. 10+ News releases related to publication #88 (Observing Nucleation in 4D), June 2019

10. 3+ News releases related to NSF Special Creativity Award and exceeding DoE targets in ORR activity by 30 times, March 2019

9. 10+ News releases related to publication #84 (Peptide Assembly and Growth on MoS2), December 2018

8. 3+ Press releases, October 2017
Following the publication of the cement force field database (CemFF) for building materials

7. 5+ Press releases, March 2017
For the award of the NASA Institute for Ultrastrong Carbon Nanomaterials (incl. CU facebook)

6. The Times (London), October 20, 2016
Mentioned as newly elected Fellow of the Royal Society of Chemistry

5. 5+ Press releases, December 2015
About the 2016 Sandmeyer Award from the Swiss Chemical Society

4. 15+ News articles, September 2015
Science Daily, Nanowerk, Spiegel Online, Materials Today, Scinexx
"Physicists determine the three-dimensional positions of individual atoms for the first time",
"Unprecedented precise determination of three-dimensional atomic positions",
"Mikroskopie Forschern gelingt Blick in dreidimensionales Atomgitter"

3. Cleveland.com/business, 2011, May 7
"Cleveland choice awards announced" (Start-up Biena Tech from my Ph.D. student KC Jha won Launchtown Award $30k)

2. Columbus Dispatch, 2011, Jan 30, p. H3
"Mimicking Mollusks - With help of supercomputer, researcher hopes to unravel how nature forms shells, teeth and bone"

1. 30+ online press releases including USA Today, Ohio Supercomputer Center, NSF 2010, December, entitled "Simulations aim to unlock nature's process of biomineralization", "Heinz accesses Ohio Supercomputing Center to study organic-inorganic binding"

Undisclosed Proprietary Work

4. Heinz, H. (for Amazon), 2023
Internal reports related to quantum computing

3. Heinz, H. (for Amazon), 2021-2023
Multiple internal reports related to grand challenge problems and solutions

2. Heinz, H. and students (for P&G), 2015-2018
Multiple internal reports for modeling of formulation components in personal care and oral care

1. Heinz, H. (for Sika AG, Zürich), 2004-2011
Multiple internal reports on modeling of organic oligomers on mineral surfaces

---

Invited Talks & Seminars (* Plenary)

231. "Using Machine Learning to Navigate the Materials Design Space" · Machine Learning in Science Workshop (TN Quantum Materials Initiative) · Middle Tennessee State University · Murfreesboro, TN · November 7, 2025

230. "Advancing Bioinspired and Low Dimensional Composite Materials Through High-Accuracy Simulations" · 13th Global Webinar on Materials Science and Engineering · November 6, 2025 (Keynote)

229. "Simulation of Energy and Functional Composite Materials Using the INTERFACE Force Field and Machine Learning" · 1st International Conference on Molecular Simulation and Intelligent Chemical Engineering · Beijing, China · November 2, 2025

228. "Accurate Force Fields for Atomistic Simulations of Oxides, Hydroxides, Multivalent Ions, and Organic Hybrid Materials up to the Micrometer Scale" · Rocky Mountain ACS Meeting (Regional) · Albuquerque, NM · October 23, 2025 (Keynote)

227. "Advancing Bioinspired and Composite MXene Materials Through High-Accuracy Simulations" · ACS Fall Meeting · Washington, DC · August 20, 2025

226. "Advancing Energy and Environmental Technologies Through High-Accuracy Simulations" · VIII Colloquium on Computational Simulation in Sciences · Universidad

Nacional Autónoma de México (UNAM) · Mexico City, Mexico · August 15, 2025 (plenary, virtual)

225. "Advancing Bioinspired and Low Dimensional Composite Materials Through High-Accuracy Simulations" · 6th International Conference on Nanospace Materials · Nagano City, Japan · July 30, 2025 (Keynote)

224. "Advancing Bioinspired and Low Dimensional Composite Materials Through High-Accuracy Simulations" · DSL Conference 2025 · Naples, Italy · June 24, 2025

223. "Integrating Simulation and Experiment to Understand Biomolecular Recognition and Nanostructure Assembly" · Institute Pasteur · Paris, France · June 23, 2025

222. "Molecular Simulations of Mineral–Biological Interfaces for Oral Health and Beyond" · Haleon PLC · Weybridge, London, UK · June 17, 2025

221. "Advancing Energy and Environmental Technologies Through High-Accuracy Simulations" · Interfaces for Energy and the Environment Conference · PNNL, Richland, WA · May 20, 2025

220. "Simulation of Flexible Electronics of 2D Materials and Composites up to the Microscale" · ACS Spring Meeting, San Diego · PMSE Division · Mar 24, 2025

219. "Advancing Bioinspired and Composite Materials Through High-Accuracy Simulations and AI" · Air Force Research Laboratory · Materials and Manufacturing Directorate/RX Seminar · Feb 20, 2025

218. "Design of Bioinspired Materials and Composites Using Experiments, Simulations and AI" · AFOSR Workshop on Design Thinking and Advanced Engineering for Extreme Environments · Kathmandu, Nepal · Dec 12, 2024

217.* "Understanding Structure, Reactivity, and Failure Mechanisms of Nanostructures and Composites Using Simulation and Experiment" · International Symposium on Stimuli-Responsive Materials 2024 · Windsor, CA · Oct 20, 2024 (Plenary)

216. "Precision Modeling of Composites and Sustainable Building Materials" · Chemical Engineering Department Seminar · Amal Jyothi College of Engineering · Kerala, India · Oct 18, 2024

215.* "Understanding the Recognition and Assembly of Amino Acids, Proteins, and Inorganic Nanostructures Using Simulation and Experiment" · International Conference on Advanced Nanomaterials for Sustainability 2024 · Kanjirappally · Kerala, India · Oct 18, 2024 (Plenary + Conference opening, covered by local press release)

214. "Guide to Writing Research Proposals" · NED University of Technology · Karachi, Pakistan · Oct 14, 2024 (Audience of 40+ new junior faculty)

213. "Panel Discussion: Opportunities and Challenges in AI-Accelerated and Data-Driven Design of Polymeric Materials" · ACS Fall Meeting · Denver, CO · Aug 20, 2024 (Moderator together with 6 panelists from academia, govmt, industry)

212. "Understanding the Recognition and Assembly of Amino Acids and Proteins at Nanoparticle Surfaces" · ACS Fall Meeting · Denver, CO · Aug 19, 2024

211. "AI-Accelerated Discovery of Materials: Challenges, Opportunities, and Integrated Test Cases" · CU Materials Science and Engineering Symposium · Boulder, CO · Aug 15, 2024

210. "Simulation of MXenes and Related 2D Hybrid Materials Up to the Micrometer Scale in High Accuracy" · MXene 2024 Conference · Drexel University, Philadelphia, PA · Aug 5, 2024
209. "Understanding Structure, Reactivity, and Failure Mechanisms of Nanostructures and Composites Using Simulation and Experiment" · AFRL, Materials and Manufacturing Directorate RX · Dayton, OH · July 10, 2024
208. "Understanding the Recognition and Assembly of Amino Acids, Proteins, and Inorganic Nanostructures Using Simulation and Experiment" · Izmir Institute of Technology, Department of Bioengineering · Izmir, Turkiye · July 8, 2024
207. "Accurate Atomistic Simulations of Metals, Oxides, Hydroxides, and Organic Hybrid Materials up to the Micrometer Scale" · BASF SE, Corporate Modeling and Data Science · Ludwigshafen, Germany · June 19, 2024
206. "Data-Driven Prediction of Mechanical Properties of Carbon Nanostructures, MXenes, and Polymer Composites" · ACS Spring National Meeting · New Orleans, LA · Mar 17, 2024
205. "Opportunities for Research and Nationwide Broadening Participation at the Intersection of AI and Materials Science" · Middle Tennessee Quantum Consortium Meeting · Murfreesboro, TN · Mar 1, 2024
204. "Understanding the Recognition and Assembly of Amino Acids and Proteins at Nanoparticle Surfaces" · IAAM Advanced Materials Lecture · Virtual · Mar 1, 2024 (Keynote)
203. "The Present and Future of HPC, Computational, and Data-Driven Materials Selection" · Leogang Workshop on HPC and AI (UCL/TUM) · Leogang, Austria · Jan 16, 2024
202. "Data-Driven Prediction of Hybrid Organic-Inorganic Structures" · AFRL/DMREF Workshop · Dayton, Ohio · Dec 7, 2023
201. "Design of Bioinspired Sustainable Materials from Atoms to Micrometers with Molecular Precision—Integration of Simulations, Large Data and Experiments" · MRS Fall Meeting · Boston, MA · Nov 28, 2023
200. "Understanding the Recognition and Assembly of Amino Acids and Proteins at Nanoparticle Surfaces" · Institute for Medical Physics and Biophysics · University of Leipzig, Germany · Nov 14, 2023
199.* "Sharing Experiences in Transatlantic Cooperation" · Consulate General of France · Los Angeles, CA · Oct 24, 2023
198. "Simulation and Machine Learning for Structure-Property Prediction of Organic-Inorganic Nanomaterials" · Chemistry Club, New Mexico Highlands University · Las Vegas, NM · Oct 12, 2023
197. "Precision Modeling of Building Materials from the Molecular Scale to the Microscale" · Department of Civil and Architectural Engineering · University of Miami, FL · Sep 22, 2023
196. "Simulation of Nanomaterials for Energy Conversion and Upgrading Natural Resources from Atoms to Micrometers: Models, Examples, and Applications" · National Renewable Energy Laboratory · Golden, CO · July 24, 2023
195. "Simulation of Nanomaterials and Composites from Atoms to Micrometers in Chemical Accuracy: Models, Examples, and Applications" · Northwestern University · Theoretical

and Applied Mechanics Seminar/Department of Civil and Environmental Engineering · Evanston, IL · May 25th, 2023

194. "Opportunities in Simulation-Driven Materials Design" · Texas Tech University · Lubbock, TX · April 3, 2023

193. "Simulation of Nanomaterials and Composites from Atoms to Micrometers in Order of Magnitude Higher Accuracy: Models, Examples, and Applications" · ACS Spring Meeting · Indianapolis, IN · March 27, 2023

192.* "Role of Solvent in Fuel Cell Catalysts, Ligands Assembly on Nanoparticles, and Solution Precursors for Carbon Fiber" · Int. Online Conference on Basic Sciences for Sustainable Development · University of Gdansk and Amal Jyothi College of Engr · December 17, 2022

191. "Simulation of Functional Materials from Atoms to Micrometers in High Accuracy: Models, Examples, and Applications" · Department of Chemistry/CNRS · University of Montpellier, France · December 12, 2022

190. "Role of Solvent in Fuel Cell Catalysts, Ligands Assembly on Nanoparticles, and Solution Precursors for Carbon Fiber" · DFG Cluster of Excellence (Resolve) · University of Bochum and University of Dortmund, Germany · December 6, 2022

189. "Modeling Local Stress Tensors in Materials and Reactive Simulation of Multiscale Mechanics" · 10th Int. Conf. on Multiscale Materials Modeling (MMM-10) · Baltimore, MD · October 5, 2022 (Keynote)

188. "Guidance in the Design of Batteries, Electrodes, and Catalysts from Simulation at the Nanoscale" · BASF SE · Ludwigshafen, Germany · August 18, 2022

187. "Simulation of Materials for Sustainability from Atoms to Micrometers in High Resolution" · Department of Physics · University of Freiburg, Germany · July 6, 2022

186. "Simulation of Materials for Sustainability from Atoms to Micrometers in High Resolution" · Amazon Tech Talk · Amazon · May 27, 2022

185. "Machine Learning for CNT Yarn Topology" · NASA US-COMP Institute Meeting · Virginia Commonwealth U · May 24, 2022

184. "Tools and Cyberinfrastructure for Simulation of Bionanostructures in High Resolution" · OpenKIM/ColabFit Workshop · U Minnesota/Virtual · May 18, 2022

183. "Tools and Cyberinfrastructure for Simulation of Bionanostructures in High Resolution" · Amazon/Grand Challenge · Virtual · Feb 28, 2022

182. "Predictive Modeling of Bionanomaterials from Picometers to Micrometers" · Pacifichem 2021 · Virtual · Dec 20, 2021

181.* "Molecular Recognition and Assembly of Biomaterials: Computational and Data Science Tools for Property Predictions" · International Conference on Advanced Nanomaterials (AICERA/ICAN) 2021 · Virtual · Dec 13, 2021

180. "The Interface Force Field and Integration in Community Resources" · NSF Cyberloop Workshop · Virtual · Nov 18, 2021

179. "Understanding the Working Mechanisms of Comb-Type Superplasticizers in Cement Hydration and Setting" · V-Renewable 2021 · Online · Sep 26, 2021 (Keynote)

178. „Predictive Modeling of Bionanomaterials from Picometers to Micrometers" · Vebleo Webinar Keynote Talk · Dec 10, 2020

177. „Predictive Modeling of Bionanomaterials from Picometers to Micrometers“ · IAAM Fellowship Lecture · Dec 9, 2020
176. „Predictive Modeling of Bionanomaterials from Picometers to Micrometers“ · University of Paris · France · Sep 25, 2020
175. „Modeling of Clay Minerals and Fine Particle Silicates to Understand Particle Assembly and Biomolecular Interactions“ · 4th Asian Clay Conference (ACC-2020) · Phuket, Thailand (transitioned to fully online) · Jun 9, 2020 (Keynote lecture)
174. „Predictive Modeling of Bionanomaterials from Picometers to Micrometers “ · Tsinghua University · China (online) · Jun 8, 2020
173. „Predictive Modeling of Bionanomaterials from Picometers to Micrometers“ · Michigan State University · Lansing, MI · Mar 10, 2020
172. „Predictive Modeling of Bionanomaterials from Picometers to Micrometers“ · U Illinois at Chicago · Chicago, IL · Feb 11, 2020
171. „Opportunities for AI-Driven Optimization of Biomaterials, Catalysts, and Composites from the Molecular Scale“ · NSF LIMPID/BisQue Workshop · University of California, Santa Barbara, CA · Feb 5, 2020
170. „Predictive Modeling of Bionanomaterials from Picometers to Micrometers“ · U Michigan · Ann Arbor, MI · Jan 14, 2020
169. „I-AIM: Interpretable Augmented Intelligence for Materials Design“ · HDR Project Kickoff Workshop · Organizer & Talk · OSU, Columbus, OH · Oct 25 & 26, 2019
168. „Predictive Modeling of Bionanomaterials from Picometers to Micrometers“ · MolSim Conference · Hangzhou, China · Oct 12, 2019
167. „Design of Biomaterials by Simulation and Experiment: Molecular Recognition, Assembly, and Applications“ · MS&T · Portland, OR · Oct 3, 2019
166. „Predictive Modeling of Bionanomaterials from Picometers to Micrometers“ · ACS Fall Meeting · San Diego, CA · Aug 25, 2019
165. „Understanding CNT Dispersion in Polymer Precursor Solutions and Properties of Composites from the Atomic Scale“ · Int. Conf. Compos. Mater. (ICCM-22) · Melbourne, Australia · Aug 15, 2019
164. „Predictive Modeling of Bionanomaterials from Picometers to Micrometers“ · ACerS/Bio4 · Toronto, Canada · Jul 25, 2019
163. „Predictive Modeling of Bionanomaterials from Picometers to Micrometers“ · CECAM Workshop on Biomolecular Mechanisms · Paris, France · May 16, 2019
162. „Simulation of Nanoparticle-Biomaterials Recognition and Assembly“ · University of Paris Diderot · Paris, France · May 14, 2019
161. Panel Discussion on Multiscale Modeling · ACS Spring Meeting · Orlando, FL · April 4, 2019
160. „Design of Biomaterials and Nanomaterials by Simulation and Experiment: Molecular Recognition, Assembly, and Applications“ · Dept of Physics and Soft Materials Research Center · University of Freiburg, Germany · Dec 19, 2018
159. „Discovery of Biomaterials Guided by Simulation and Experiment: Molecular Recognition, Assembly, and Applications“ · Workshop on Self-Assembly and Hierarchical Materials in Biomedicine (SAHMB) · San Sebastian, Spain · Oct 9, 2018

158. „Design of Composites, Catalysts, and Building Materials Using Insights from Simulation and Experiment“ · MCM’18 Congress · Madrid, Spain (via Webex) · Aug 16, 2018 (Keynote Talk)
157. „Understanding Mineral-Water Interfaces“ · Gordon Conf. Biomineralization · Colby Sawyer College, NH · July 29, 2018 (Discussion Leader)
156. „Carbon Nanotube Dispersion in Polymer Solutions and Nanoscale Properties of Polyacrylonitrile/CNT Composites“ · AFRL/RX · Dayton, Ohio · July 25, 2018
155. „Design of Biomaterials and Nanomaterials by Simulation and Experiment: Molecular Recognition, Assembly, and Applications“ · BASF · Ludwigshafen, Germany · July 17, 2018
154. „Understanding Multiphase Materials Interactions from Molecules to Microstructures“ · University of Mainz, Department of Physics · Mainz, Germany · Jun 21, 2018
153. „A C-S-H Builder and Interface Modeling Tools for Accurate Full Electrolyte Simulations“ · Workshop on Calcium Aluminum Hydrates in Cement · EMPA, Dubendorf, Switzerland · Apr 23/24, 2018
152. „Design and Testing of Nanoalloy Catalysts in 3D Atomic Resolution“ · NSF/DoE/AF Materials Genome Initiative PI Meeting · U Maryland, MD · Mar 26, 2018
151. „Discovery of Biomaterials by Simulation and Experiment: Catalysts, Composites, and Therapeutics“ · TMS National Meeting · Phoenix, AZ · Mar 12, 2018
150. „Precision Modeling of Building Materials: Understanding Multiphase Material Interactions and Mechanics from Molecules to Civil Structures“ · ETH Zurich, Department of Civil Engineering · Zurich, Switzerland · Jan 9, 2018
149. „Discovery of New Materials by Simulation and Experiment: From Molecular Recognition to Catalysts, Composites, and Therapeutics“ · Nanyang Technological University, Materials Science and Engineering · Singapore · Nov 10, 2017
148. „Discovery of New Materials by Simulation and Experiment: From Molecular Recognition to Catalysts, Composites, and Therapeutics“ · Natl University of Singapore, Department of Chemistry · Singapore · Nov 9, 2017
147. „Discovery of New Materials by Simulation and Experiment: From Molecular Recognition to Catalysts, Composites, and Therapeutics“ · A*Star, Institute for High Performance Computing · Singapore · Nov 8, 2017
146. „Molecular Details of Photorepsonses of Switchable Azobenzene Derivatives and Alkylammonium Surfactants in Clay Interlayer Spaces“ · 16th Int. Clay Conf. · Granada, Spain · July 18, 2017 (Keynote Talk)
145. „Molecular Modelling of Clays and Related Materials Using Empirical Interatomic Potentials / IFF“ · AIPEA School for Young Scientists · Granada, Spain · July 15/16, 2017 (Invited Lecture and Tutorial)
144.* „Discovery of New Materials by Simulation and Experiment: From Molecular Recognition to Catalysts, Composites, and Therapeutics“ · Int. Conf. on Emerging Areas in Materials Engineering · Amal Jyothi Coll. Engr, Kerala, India · July 13, 2017
143. „Reliable Computational Design of Biological-Inorganic Materials to the Large Nanometer Scale Using INTERFACE-FF“ · Fritz-Haber Inst of the Max-Planck Society · Berlin, Germany · June 22, 2017

142. „Molecular Principles of Green Nanomaterials Recognition and Assembly from Molecular Simulations“ · ACS Green Chemistry Conference · Reston, VA · June 15, 2017 (by Krishan Kanhaiya)
141. „Reliable Computational Design of Biological-Inorganic Materials“ · CECAM Workshop · Bremen, Germany · June 14, 2017
140.* “Discovery of New Materials by Simulation and Experiment: From Molecular Recognition to Catalysts, Composites, and Therapeutics“· Bilkent University Nanoday · Ankara, Turkey · May 25, 2017
139. “Insight into Clay/Water Interfaces and Applications to Nanomaterials“ · Middle East Technical University, Geol. Engr. · Ankara, Turkey · May 24, 2017
138. “Explaining Cement Chemistry Using the INTERFACE Force Field: Foundations, Parameters, Surface Models, and Application“ · Nanocem Workshop · Les Diablerets, Switzerland · May 18, 2017
137.* “Development of Commercial Organic Additives for the Grinding of Inorganic Solids“ · SCS 13th Freiburger Sympsium · Fribourg, Switzerland · May 12, 2017
136. “Simulation of Biological and Nanostructured Interfaces to Discover New Materials“ · IEEE-NEMS · UCLA, Los Angeles, CA · Apr 12, 2017
135. „Reliable Computational Design of Biological-Inorganic Materials to the Large Nanometer Scale Using INTERFACE-FF“ · ACS Spring Meeting · San Francisco, CA · Apr 4, 2017
134. „Computational Design of Biological-Inorganic Materials from the Nanoscale“ · Lonza AG · Visp, Switzerland · Mar 13, 2017
133. „Computational Design of Biological-Inorganic Materials from the Nanoscale“ · TMS National Meeting · San Diego, CA · Feb 28, 2017
132. „Reliable Computational Design of Biological-Inorganic Materials to the Large Nanometer Scale Using INTERFACE-FF“ · ICMS-2016 · Shanghai, China · Oct 24, 2016
131. „Rational Design of Mechanical Properties of Polyacrylonitrile Carbon Fibers“ · AFOSR Low Density Materials Review · Arlington, VA · Oct 13, 2016 (with Satish Kumar)
130. „Computational Design of Biological-Inorganic Materials to the Large Nanometer Scale Using INTERFACE-FF“ · CECAM School on Soft Matter Simulation · Schloss Waldthausen, Germany · Oct 12, 2016 (1.5 h Lecture + Tutorial)
129.* „Clay/Water Interfacial Models (Kaolinite, Micas, Montmorillonite) to Reproduce Contact Angles and Organic Adsorption“ · 5th Mediterranean Clay Meeting · Cesme/Izmir, Turkey · Sep 26, 2016 (Plenary after opening ceremony)
128.* “Development of Commercial Organic Additives for the Grinding of Inorganic Solids” · Sandmeyer Award Lecture, Swiss Chemical Society Fall Meeting · Zurich, Switzerland · Sep 15, 2016
127. “Simulation of Biological and Nanostructured Interfaces to Discover New Materials“ · Research Seminar, Adolphe Merkle Institute · Fribourg, Switzerland · Sep 13, 2016
126. “The INTERFACE Force Field and a Surface Model Database“ · Workshop on Integrated Simulation of Bio and Nanomaterials · Lehigh U, PA · Aug 24, 2016
125. “Simulation of Silicate and Aluminate Interfaces with Organic Additives, Water, and Alloys as a Function of Composition and pH” · Research Seminar, Corning · Corning, NY · Aug 4, 2016

124. “Nanoscale Modeling of Ni-Cr-Al and Mo-Si Oxidation and Interfacial Properties“ · ONR Program Review, UVa · Charlottesville, VA · Jun 29, 2016
123. “Simulation of Biological and Nanostructured Interfaces to Discover New Materials“ · CC3DMR Conference · Incheon, Korea · Jun 21, 2016
122. “Mechanism of Molecular Interaction of Superplasticizer Oligomers with Hydrated Cement Phases” · ETH Zurich, Dept of Civil Engr · Zurich, Switzerland · Jun 20, 2016 (by Tariq Jamil)
121. “Mechanism of Specific Recognition of Pt Nanocrystals by Peptides and of their Formation from Seed Crystals“ · BIOMATSEN Conference · Istanbul, Turkey · Jun 2, 2016
120. “Simulation of Biological and Nanostructured Interfaces to Discover New Materials“ · APMAS Conference · Istanbul, Turkey · Jun 1, 2016
119. “FATENANO: Simulation of Biological and Nanostructured Interfaces to Understand Biological Fate“ · CIC Biomagune · San Sebastian, Spain · May 26, 2016
118. “Forcefield Improvements for CNT/Matrix Interactions and Nature of Polyacrylonitrile-CNT Interactions“ · Structural CNT Working Group Meeting · NASA Langley Res Ctr, VA · Apr 28, 2016
117. “Simulation of Biological and Nanostructured Interfaces to Discover New Materials“ · Global Nanotech Conf & Expo 2016 · Dubai, UAE · Apr 23, 2016
116. “Nanoscale and Multi-Scale Approaches to Design Building Materials“ · Global Nanotech Conf & Expo 2016 · Dubai, UAE · Apr 21, 2016
115. “Simulation of Biological and Nanostructured Interfaces to Discover New Materials“ · EMN Meeting · Kona, HI · Mar 22, 2016
114. “Prediction of Surface and pH-Specific Binding of Polymers and Biomacromolecules to Metal and Oxide Nanostructures Using Computational Models“ · ACS Spring Meeting · San Diego, CA · Mar 15, 2016
113. “Mechanism of Specific Recognition of Pt Nanocrystals by Peptides and of their Formation from Seed Crystals“ · TMS National Meeting · Nashville, TN · Feb 16, 2016
112. “Simulation of Biological and Nanostructured Interfaces to Discover New Materials“ · University College London, Department of Chemistry · London, UK · Jan 4, 2016
111. “Mechanisms of Molecular Recognition and Assembly at the Nanoscale: Computation Meets Experiment“ · University of Miami, Department of Chemistry · Miami, FL · October 23, 2015
110. “Prediction of Surface and pH-Specific Binding of Peptides to Metal and Oxide Nanoparticles“ · ACS Fall Meeting · Boston, MA · August 16, 2015
109. “Simulation of Polymer-Inorganic Interfaces and Assembly at the Nanoscale: Computation Meets Experiment“ · Corning · Corning, NY · August 11, 2015
108. “Mechanisms of Molecular Recognition and Assembly at the Nanoscale: Computation Meets Experiment“ · Shanghai Jiao Tong University · Shanghai, China · Apr 29, 2015
107. “Mechanisms of Molecular Recognition and Assembly at the Nanoscale: Computation Meets Experiment“ · Analytix2015 · Nanjing, China · Apr 26, 2015
106. “Mechanisms of Molecular Recognition and Assembly at the Nanoscale: Computation Meets Experiment“ · IUPUI, Chemistry · Indianapolis, IN · Apr 22, 2015

105. "Insight into Nanoscale Properties of Polymers and Hydrogels from Molecular Simulation" · Eastman Chemical · Kingsport, TN · Apr 16, 2015
104. "Mechanisms of Molecular Recognition and Assembly at the Nanoscale: Computation Meets Experiment" · Northeastern University, Chemical Engineering · Boston, MA · Mar 17, 2015
103. "Mechanisms of Molecular Recognition and Assembly at the Nanoscale: Computation Meets Experiment" · Akron Section of ACS · Akron, OH · Feb 18, 2015
102. "Mechanisms of Molecular Recognition and Assembly at the Nanoscale: Computation Meets Experiment" · Virginia Tech, Chemical Engineering · Blacksburg, VA · Feb 6, 2015
101. "Mechanisms of Molecular Recognition and Assembly at the Nanoscale: Computation Meets Experiment" · University of Colorado-Boulder, Chemical and Biological Engineering · Boulder, CO · Jan 27, 2015
100. "The INTERFACE Force Field for the Accurate Simulation of Inorganic, Organic, and Biomolecular Compounds in a Single Platform" · Biovia/Dassault Systemes · Webinar for Materials Community · Nov 13, 2014
99. "Atomic-Scale Structure and Catalytic Functionality of Bio-Inspired Nanoparticles: A Systematic Approach Using Computation and Experiment" · MS&T 2014 · Pittsburgh, PA · Oct 15, 2014 (by H. Ramezani-Dakhel)
98. "Bioinspired and Layered Oxide Materials for Renewable Energy and Therapeutics: Insight from Molecular Models and Simulations at the 1-100 Nanometer Scale" · International Center for Materials Nanoarchitectonics (MANA) · National Institute for Materials Science (NIMS), Tsukuba, Japan · June 17, 2014
97. "Tutorial: How to Use the INTERFACE Force Field, Connect with Laboratory Tests and Multi-Scale Simulation Methods" · NSF Workshop on Transformative Technologies in Molecular Simulation · University of Wisconsin, Madison, WI · May 19, 2014
96. "The INTERFACE Force Field to Unite Materials and Biomolecular Simulation in a Single Platform: Examples of Protein Recognition on Metals, Silicates, and Phosphates" · NSF Workshop on Transformative Technologies in Molecular Simulation · University of Wisconsin, Madison, WI · May 19, 2014
95. "Challenges for Force Fields of Clay Minerals and New Kaolinite Parameters" · Clay Minerals Society · College Station, TX · May 18, 2014
94. "Molecular Modeling of Multiphase Hydrogels for Particle Suspensions" · Procter and Gamble · Cincinnati, OH · May 14, 2014
93. "Nanoscale pH-Responsive Interfaces of Hydroxyapatite - Molecular Modeling of Sn2+/Zn2+ Interaction with Enamel and Formulation Ingredients" · Procter and Gamble · Cincinnati, OH · May 13, 2014
92. "Understanding Nanoscale pH-Responsive Interfaces of Hydroxyapatite and Silica for Selective Interactions with Peptides and Drug Molecules" · 6th Scientific Readings "A Modern Cement Plant" · Moscow, Russia · Nov 26, 2013
91. "Hybrid Solid-State Photovoltaic Materials and Devices" · US/Mexican Basic Research Initiative Final Workshop · Ensenada, MX · Sep 18, 2013

90. "Understanding Nanoscale pH-Responsive Interfaces of Hydroxyapatite and Silica for Selective Interactions with Peptides and Drug Molecules" · ACS National Meeting (D-COLL) · Indianapolis, IN · Sep 12, 2013
89. "Compatibility of Force Fields for Different Materials Classes and Validation of Interfacial Properties:The Interface Force Field as an Integrated Approach" · NIST Workshop on Interatomic Potentials for Industrial Needs · NIST, Gaithersburg, MD · August 14, 2013
88. "Metals, Silicates and Phosphates in Nanobiotechnology: From Nanoscale Interfaces to Applications" · Condensed Matter Theory Seminar, University of Mainz · Mainz, Germany · July 9, 2013
87. "Specific Adsorption of Grinding Aids and Molecules on Cement Phases and Silica" · Sika AG · Zurich, Switzerland · July 5, 2013
86. "Mechanisms of Molecular Recognition and Shape Control at the Nanoscale: Computation Meets Experiment" · CECAM Workshop on Solid-Liquid Interfaces · Lausanne, Switzerland · June 25, 2013
85.* "Silicates and Phosphates in Nanobiotechnology: From Nanoscale Interfaces to Applications" · Minerals for Life, Mineralogical Society · Edinburgh, UK · June 18, 2013
84. "Understanding Molecular Recognition and Growth of Metal Nanostructures from a Molecular Perspective" · University of Durham, Department of Chemistry · Durham, UK · June 10, 2013
83. "Structure, Dynamics, and Cohesion of Clay Intercalation Compounds with Functional Surfactants" · International Symposium on Materials Chemistry of Intercalation Compounds (MCIC2013) · Tokyo, Japan · May 11, 2013
82. "Aqueous Interfacial Properties of Silica, Cement Minerals, and Hydroxyapatite in Comparison to Clay Minerals" · Waseda University · Tokyo, Japan · May 9, 2013
81. "Mechanisms of Molecular Recognition and Self-Assembly at the Nanoscale: Computation Meets Experiment" · Department of Chemical Engineering, Auburn University · Auburn, AL · March 25, 2013
80. "Mechanisms of Molecular Recognition and Self-Assembly at the Nanoscale: Computation Meets Experiment" · School of Chemistry, Georgia Institute of Technology · Atlanta, GA · February 5, 2013
79. "Mechanisms of Molecular Recognition and Self-Assembly at the Nanoscale: Computation Meets Experiment" · Department of Materials Science and Engineering, University of California – Los Angeles · Los Angeles, CA · January 25, 2013
78. "Mechanisms of Molecular Recognition and Self-Assembly at the Nanoscale: Computation Meets Experiment" · SERMACS · Raleigh, NC · November 15, 2012
77. "Mechanisms of Molecular Recognition and Self-Assembly at the Nanoscale: Computation Meets Experiment" · Ohio Supercomputing Center, Ohio State University · Columbus, OH · November 2, 2012
76. "Clay Minerals for Nanocomposites and Biotechnology: Surface Modification, Dynamics, and Responses to Stimuli" · Clay Minerals Society Annual Meeting · Golden, CO · July 11, 2012

75. "Mechanisms of Molecular Recognition and Self-Assembly at the Nanoscale: Computation Meets Experiment" · California Institute of Technology, Chemistry and Chemical Engineering · Pasadena, CA · July 5, 2012
74. "Mechanisms of Molecular Recognition and Self-Assembly at the Nanoscale: Computation Meets Experiment" · University of Strathclyde, Chemical Engineering · Glasgow, UK · May 24, 2012
73. "Mechanisms of Molecular Recognition and Self-Assembly at the Nanoscale: Computation Meets Experiment" · University of Mainz (Physics) · Mainz, Germany · May 4, 2012
72. "Insight into Molecular Recognition and Mechanical Properties at the Nanoscale Using Computational Approaches" · Army Research Laboratory (Materials and Manufacturing Directorate) · Aberdeen Proving Ground, MD · Apr 25, 2012
71. "Force Field Parameters for Interfaces: Silicates and Hydroxides" · Accelrys, Inc. · San Diego, CA · Mar 30, 2012
70. "Mechanism of Adsorption of Peptides and Surfactants on Metal Surfaces" · ACS Spring Meeting (D-COLL) · San Diego, CA · Mar 27, 2012
69. "Understanding of Molecular Recognition and Self-Assembly at the Nanoscale Using Computational Tools" · Materials Science and Engineering Program · Sabanci University · Istanbul, Turkey · Mar 14, 2012
68. "Organic and Hybrid Organic Solid-State Photovoltaic Materials and Devices: Modeling and Simulation of Interfacial Dynamics" · AFOSR/MX Basic Research Initiative · Wright-Patterson AFB · Dayton, OH · Feb 8, 2012
67. "Understanding Size Control and Catalytic Performance of Peptide-Capped Pd Nanoparticles Using Simulation" · Biotechnology Review · Air Force Research Laboratory · Dayton, OH · Jan 17, 2012
66. "Computer-Aided Understanding of Molecular Recognition and Self-Assembly at the Nanoscale" · Adolphe Merkle Institute Fribourg, Switzerland · Dec 12, 2011
65.* The George Brown Lecture of the Mineralogical Society of Great Britain and Ireland: "Clay Minerals for Nanocomposites and Biotechnology: Surface Modification, Dynamics, and Responses to Stimuli" · Euroclay 2011 · Antalya, Turkey · Jun 27, 2011
64. "Understanding and tuning the binding strength of surfactants and biomolecules to Au and Pd surfaces in solution: Molecular epitaxy, covalent bonding, and induced charges" · CMOS Emerging Technologies Workshop · Hilton Resort and Spa · Whistler, CA · Jun 17, 2011
63. "Understanding Biomolecule-Inorganic Interfaces and Growth of Anisotropic Nanostructures" · NSTI Nanotech 2011 · Boston, MA · Jun 14, 2011
62. "Challenges and Opportunities for Nanomaterials Chemistry and Biology in Silico" · ETH Zurich, Department of Civil Engineering · Zurich, Switzerland · Jun 9, 2011
61. "Molecularly Designed Interfaces for Construction Materials, Sensors, and Catalysts: From Theory to Applications" · ETH Zurich, Deprtament of Civil Engineering · Zurich, Switzerland · Jun 6, 2011
60. "Molecular-Level Understanding of Biomolecule-Inorganic Interactions" · CECAM Workshop "Grand Challenges in Understanding Interfaces Between Hard and Soft Matter" · EPFL Lausanne · Switzerland · May 11, 2011

59. "Molecularly Designed Interfaces for Biomaterials, Sensors, and Catalysts: From Theory to Applications" · University of Washington · Department of Materials Science and Engineering · Seattle, WA · Apr 18, 2011
58. "Molecularly Designed Interfaces for Biomaterials, Sensors, and Catalysts: Force-field Based Simulation and New Theory" · Center for Advanced Scientific Computing and Modeling · University of North Texas · Denton, TX · Apr 7, 2011
57. "Molecular-Level Understanding of Biomolecule-Inorganic Interactions" · Exploring Biological Interfaces Workshop · Caribe Hilton Hotel · San Juan, PR · Apr 4-6, 2011
56. "Simulation of Biomaterials and Interfaces" · Institute of Materials Science · University of Jena · Jena, Germany · Feb 14, 2011
55. "Binding of Peptides to Metal and Silica Nanostructures - Relation between Particle Size, Peptide Sequence, and Catalytic Activity" · AFRL Biotech Review · WPAFB, OH · Jan 12, 2011 (delivered by R. J. Berry due to weather).
54. "Selective Adsorption of Biomolecules on Nanostructured Metal and Silica Surfaces" · Department of Physics · University of Mainz, Germany · Dec 17, 2010
53. "NSF Career: Unraveling Molecular Mechanisms of Biomineralization" · Board of Trustees Meeting · University of Akron, OH · Dec 15, 2010
52. "Nanomechanics and Dispersion of Layered Silicates in Polymer Matrices" · 2nd Int. Conf. on Nanomechanics and Nanocomposites · Beijing, China · Oct 11, 2010
51. "A Model for CSH with Validated Structural and Surface Properties" · Sika Technology AG · Zurich, Switzerland · June 30, 2010
50. "Molecular Models and Methods to Understand Self-Assembly of Inorganic-Bioorganic Multiphase Materials" · NSTI Nanotech 2010 · Anaheim, CA · June 22, 2010
49. "Interaction of Protein Building Blocks and Surfactants with Shaped Surfaces of Au, Pd, and Silica in Aqueous Solution" · CERMACS 2010 · Dayton, OH · June 16, 2010
48. "Interaction of Protein Building Blocks and Surfactants with Shaped Surfaces of Au, Pd, and Silica in Aqueous Solution" · Institute for Complex Adaptive Matter, JNC for Adv Sci Res · Bangalore, India · April 26, 2010
47. "Interaction of Protein Building Blocks and Surfactants with Shaped Surfaces of Au, Pd, and Silica in Aqueous Solution" · Telluride Workshop on Interfacial Phenomena in Nanostructured Materials and Devices · Telluride, CO · Feb 10, 2010
46. "Molecular Simulation of Adsorption of Protein Building Blocks and Surfactants on Shaped Metal and Silicate Surfaces in Aqueous Solution" · Max-Planck Inst. for Dyn. Comp. Techn. Syst. · Magdeburg, Germany · Jan 8, 2010
45. "Force Field Development for Layered Silicates, FCC Metals, Polymers, and Their Application" · Accelrys, Inc. · Cambridge, UK · Nov 9, 2009
44.* "Interaction of Peptides and Surfactants with Shaped Surfaces of Au, Pd, and Silica in Aqueous Solution" · Int. Symp. Stim. Resp. Materials · Hattiesburg, MS · Oct 28, 2009
43. "Nanoscale Linear Mechanical and Cleavage Properties of Layered Silicates" · Sandia National Laboratories · Albuquerque, NM · Sep 22, 2009
42. "Interaction of Protein Building Blocks and Surfactants with Shaped Surfaces of Au, Pd, and Silica in Aqueous Solution" · AFRL/RX Biotech Review, WBI · Dayton, OH · Sep 15, 2009

41. "Interaction of Protein Building Blocks and Surfactants with Shaped Surfaces of Au and Pd Nanostructures in Solution" · University of Akron, Department of Polymer Science · Akron, OH · Sep 3, 2009
40. "Functional Interfaces of Silicates with Peptides and Polymers Guided By Molecular Simulation" · ACS Fall National Meeting · Washington, DC · August 19, 2009
39. "Interaction of Protein Building Blocks and Surfactants with Shaped Surfaces of Au and Pd Nanostructures in Solution" · University of Patras (Greece)· Department of Chemical Engineering · June 29, 2009
38. "Interaction of Amino Acids, Surfactants, and Peptides with Even, Stepped, and Spherical Surfaces of Gold and Palladium Nanostructures in Aqueous Solution" · AFRL/RX Research Meeting· Wright-Patterson AFB, OH · May 29, 2009
37. "Simulation of FCC Metals and Metal-Biological Interfaces for Nanoelectronic and Sensor Applications" · NIST · Workshop on Atomistic Simulations for Industrial Needs · Gaithersburg, MD · Apr 27, 2009
36. "Design of Functional Nanoparticle Interfaces and Polyelectrolytes Guided By Atomistic Simulation" · Int. Conf. on High Tech Mat. 2009 · IIT Kharagpur, India · Feb 12, 2009
35. "Molecular Dynamics Simulation of Poly(ethylene oxide) and Clay Mineral Interfaces with Surfactants and Peptides In Aqueous Solution" · Procter & Gamble · Cincinnati, OH · · Dec 19, 2008
34. "Modeling the Interaction of Peptides and Surfactants with Inorganic Surfaces: Understanding Specificity Through Computation and Experiment" · Dept Seminar Chemistry · Nottingham Trent Univ · Nottingham, UK · Nov 5, 2008
33. "Adsorption of Single Amino Acids and Surfactants to Au {111} Surfaces in Aqueous Solution - Insight from Atomistic Simulation" · Dept Seminar Physics · Univ of South Mississippi, MS · Oct 31, 2008
32.* "Design of Functional Nanoparticle Interfaces and Polyelectrolytes Guided By Atomistic Simulation" · Int. Conf. on Stimuli-Responsive Materials · Hattiesburg, MS · Oct 29, 2008
31. "Nanomechanics and Energetics of Layered Silicates for Nanocomposites" · ACS Rubber Tech Meeting and Expo · Louisville, KY · Oct 15, 2008 (given by J. Feng)
30. "Simulation of Metals and Metal-Biological Interfaces for Sensor and Nanoelectronic Applications" · Dept Seminar Math and Applied Math · Univ of Akron, OH · Oct 2, 2008
29. "Atomistic Simulation of PEO in Solution – Challenges and New Models" · University of Mainz, Germany · Condensed Matter Physics Seminar · June 24, 2008
28. "Peptide Binding to Inorganic Surfaces and Thermal Transitions of Alkyl Chains on Nanoparticle Surfaces: Computation and Experiment" · ACS Central Regional Meeting · Columbus, OH · June 11, 2008
27. "Simulation of Inorganic-(bio)organic Interfaces and Thermal Transitions of Alkyl Chains on Surfaces" · Smart Coatings 2008 · Orlando, FL · Feb 27, 2008
26. "Molecular Simulation of Inorganic-Biological Interfaces and Optically Switchable Materials" · 7th Int. Conf. on Adv. Polymers for Macromol. Eng. (APME) · Miami, FL · Dec 17, 2007
25.* "Atomistic Simulation of Inorganic-Biological Interfaces and Optically Switchable Materials" · 2nd International Symposium on Stimuli-Responsive Materials · University of Southern Mississippi · Hattiesburg, MS · Oct 31, 2007

24. “Peptide Binding to Sheet Silicate and Metal Nanonoparticles − Insight from Atomistic Simulation” · SAMPE Fall Technical Meeting · Cincinnati, OH · Oct 30, 2007
23. “Effective Atomistic Models for Inorganic-Biological Interfaces and Optically Switchable Materials” · Kent State University, Dept of Chemistry · Kent, OH · Sep 06, 2007
22. “Influence of Peptide Sequence on Adsorption on Au, Pd, and Montmorillonite Nanoparticle Surfaces - Insight from Atomistic Simulation” · WPAFB, AFRL/ML, Dayton, OH · Aug 14, 2007
21. “A Force Field for Layered Silicates and Simulation of Interfaces with Surfactants and Peptides” · 44th Annual Meeting of the Clay Minerals Society · Santa Fe · NM · June 6, 2007
20. “Simulation of Hybrid Materials and Interfaces: Insight from Atomistic and Coarse-grain Models” · ORNL · Chemical Sciences Division · Knoxville, TN · Mar 6, 2007
19. “Peptide Design for Binding to Metal Surfaces Using Atomistic Simulation” · WPAFB, AFRL/ML, Dayton, OH · Feb 20, 2007
18. “Force Fields for Sheet Silicates and Metals” · Accelrys User Meeting and Conference Baltimore, MD · Nov 15, 2006
17. ”Simulation of Nanostructured Materials Using Atomistic and Coarse Grain Models” University of Central Florida · Nanoscience and Technology Center · Orlando, FL · Apr 26, 2006
16. ”Simulation of Nanostructured Materials Using Atomistic and Coarse Grain Models” University of Akron · Dept. of Polymer Engineering · Akron, OH · Apr 18, 2006
15. ”Simulation of Nanostructured Materials Using Atomistic and Coarse-Grain Models” Florida State University · Dept. of Chemical and Biomedical Engineering · Tallahassee, FL · Mar 14, 2006
14. “Simulation of Organic-Inorganic Interfaces Containing Sheet Silicates” · Los Alamos National Laboratory · Theory Division · Los Alamos, NM · Feb 15, 2006
13. “Simulation of Organic-Inorganic Interfaces Using Atomistic and Coarse Grain ModelsAcademia Sinica · Research Center for Applied Sciences · Taipei, Taiwan · Feb 9, 2006
12. ”Simulation of Organic-Inorganic Interfaces Using Atomistic and Coarse Grain Models” University of Karlsruhe · DFG Center for Functional Nanomaterials · Karlsruhe, Germany Jan 18, 2006
11. ”Atomistic Simulation of Nanostructured Interfaces with Sheet Silicates” · University of Mainz · Department of Physics · Condensed Matter Theory Seminar · Dec 22, 2005
10. ”Towards Quantitative Atomistic Simulation of Nanostructured Hybrid Materials” · UIUC Department of Physics (Yia-Chung Chang) · Nov 9, 2005
9. "Simulation of Structure-Property Relationships in Polymer/Layered Silicate Nanocomposites" · ACS Rubber Expo, Fall 168th Technical Meeting · Pittsburgh, PA · Nov 1, 2005
8. "Self-assembly of alkylammonium chains on montmorillonite: Effect of chain length, head group structure, and cation exchange capacity" · AFRL/ML, WPAFB · Polymer Branch Research Seminar · Oct 7, 2005
7. “Molecular Modeling of Superplasticizers in Cementitious Systems: Progress” · Sika Technology AG · Zurich, Switzerland · Apr 12, 2005

6. “Energy Models and Atomistic Simulation of Clays with Surface-Grafted Alkylammonium Chains” · MIT · Atomistic Modeling and Simulation Seminar (AMASS) Cambridge, MA · Nov 29, 2004
5. "Modeling Single Molecule Spectral Shifts and Organically Modified Silicates" · ETH Zurich, Swiss Center for Scientific Computing · Computational Chemistry Seminar (M. Parrinello) · Manno, Switzerland · Sep 24, 2003
4. "Simple Energy Models and Simulation of Organically Modified Silicates" · University of Akron · Department of Polymer Science · Polymer Science Colloquium · Aug 19, 2003
3. "Simple Energy Models and Simulation of Organically Modified Silicates" · Air Force Research Laboratory, Wright-Patterson AFB · Materials Science and Technology Colloquium · Dayton, OH · Aug 15, 2003
2. "Partial Charges in Polar Solids" · University of Mainz · Department of Physics · Seminar on Condensed Matter Theory · Mainz, Germany · Dec 3, 2002
1. “Molecular Modeling of Dye-doped Hydrocarbons” · ETH Zurich · Institute of Quantum Electronics · Group Seminar Prof. H. Baltes · Zurich · Jan 20, 2001

Conference Contributions (Talks, Posters incl. coworkers, incomplete)

226.T “Atomistic Simulations of Oxides, Hydroxides, and Electrolyte / Organic Interfaces Up to the Large Nanometer Scale” · U Bochum, Physics · Bochum, Germany · January 8, 2026

225.T “Prediction of Carbon Nanostructure Mechanical Properties and the Role of Defects Using Machine Learning” · Rocky Mountain ACS Meeting (Regional) · Albuquerque, NM · October 25, 2025

224.T “Opportunities and Challenges in Materials Simulation and AI-driven Methods” · Lunch & Learn · ChBE, CU Boulder · Sep 26, 2025

223.P “Shear Simulations of MXenes” · AFRL/RX · Dayton, Ohio · Aug 15, 2025 (by Sean Florez)

222.T “Parameters for Aqueous Ions” · BASF SE · Ludwigshafen, Germany · June 27, 2025

221.P “Utilizing Machine Learning in Predicting Perovskite Structure” · ACS Fall Meeting · Denver, CO · Aug 20, 2024 (by William Ashcraft)

220.P “Molecular Mechanisms and Design Principles of CO2 Absorption and Volatility in Ionic Liquid Mixtures” · ACS Fall Meeting · Denver, CO · Aug 20, 2024 (by Isaac Armstrong)

219.T “Accurate Force Fields for Atomistic Simulations of Oxides, Hydroxides, and Organic Hybrid Materials up to the Micrometer Scale” · ACS Fall Meeting · Denver, CO · Aug 20, 2024

218.T “Interface Force-Field (IFF) Parameterization of Ti3C2TX MXenes and Prediction of Nanoscale Shear Properties” · ACS Fall Meeting · Denver, CO · Aug 19, 2024 (by Isaac Armstrong)

217.T “Coarse-Grained MD Simulations of Protein Binding to Nanoparticle Surfaces: Effect of Complex Biological Media on Drug Targeting” · ACS Fall Meeting · Denver, CO · Aug 19, 2024 (by Miryana Hemadi)

216.P "Molecular Dynamics Simulation and Machine Learning Prediction of Structures of Hybrid Organic Inorganic Perovskites" · ACS Fall Meeting · Denver, CO · Aug 19, 2024 (by Leo Beck and Isaac Armstrong)

215.T "Implementation of Reactivity in Molecular Dynamics Simulations Using Classical Force Fields" · ACS Fall Meeting · Denver, CO · Aug 18, 2024 (by Jordan Winetrout)

214.P "CSSI Framework: Cyberloop for Accelerated Bionanomaterials Design" · NSF Cyberinfrastructure and Cybertraining PI Meeting · Charlotte, NC · August 12, 2024

213.P "Data-Driven Prediction of Hybrid Organic-Inorganic Structures" · NSF Materials Genome Initiative PI Meeting · Washington, DC · July 30, 2024

212.T "Understanding the Recognition and Assembly of Amino Acids, Proteins, and Inorganic Nanostructures Using Simulation and Experiment" · AFRL, Materials and Manufacturing Directorate RX (Rajiv Berry's team) · Dayton, OH · July 26, 2024

211.T "Understanding Mechanical Behavior of MXenes for Structural Multi-Functional Composites via Multiscale Modeling" · ACS Spring National Meeting · New Orleans, LA · Mar 17, 2024 (by Vikas Varshney, AFRL)

210.P "AI-Driven Design of 2D Materials, Polymer, and Electrolyte Interfaces for Accelerated Design of Composites and Sensors" · 2024 GRC on Multifunctional Materials · Ventura, CA · Jan 29/30, 2024

209.T "Nonbonded Models to Simulate FCC Metals, Metal Oxides, Metal Hydroxides, and Their Applications" · Leogang Workshop on HPC and AI (UCL/TUM) · Leogang, Austria · Jan 16, 2024 (by Krishan Kanhaiya)

208.P "Atomic Resolution of the ALD Li-Al-O Film Nanostructure on Li-Ion Layered Cathode Oxides" · 2023 AIChE Annual Meeting · Orlando, FL · Nov 6, 2023 (by Julie Ngyuen, HH, and Al Weimer)

207.T "Ultrathin: Understanding the Nanostructure of Alumina Atomic Layer Deposited Films on Layered Cathode Oxides" · 2023 AIChE Annual Meeting · Orlando, FL · Nov 6, 2023 (by Julie Ngyuen, HH, and Al Weimer)

206.P "CSSI Framework: Cyberloop for Accelerated Bionanomaterials Design" · 2023 NSF CSSI PI Meeting · Houston, TX · Sep 26, 2023

205.T "A Comparative Study of Machine Learning Techniques for Carbon Nanostructure Mechanical Properties" · NASA US-COMP Institute Meeting · Richmond, VA and Virtual · May 9, 2023 (by Jordan Winetrout and Hendrik Heinz)

204.T "Seeing Single Atoms in Materials Via Atomic Electron Tomography" · AIChE National Meeting · Phoenix, AZ · Nov 18, 2022 (by Saman Moniri, Hendrik Heinz, Jianwei Miao, et al.)

203.P "Unveiling the Surface Molecular Pump Effect of DMF on Pt-Based ORR Catalysts By Molecular Dynamics Simulations" · AIChE National Meeting · Phoenix, AZ · Nov 17, 2022 (by Cheng Zhu and Hendrik Heinz)

202.T "Prediction of Metal-Organic Interactions and Molecular Assembly in High Accuracy and Speed" · AIChE National Meeting · Phoenix, AZ · Nov 16, 2022 (by Cheng Zhu and Hendrik Heinz)

201.P "Modeling Perovskites for Solar Energy Harvesting Using Molecular Dynamics Simulations" · AIChE National Meeting · Phoenix, AZ · Nov 15, 2022 (by Barbara Morales and Hendrik Heinz)

200.P "Explaining Improvements in Li-ion Battery Performance By Atomic Layer Deposition of Alumina Using Molecular Dynamics Simulation" · AIChE National Meeting · Phoenix, AZ · Nov 15, 2022 (by Julie Ngyen, Al Weimer, and Hendrik Heinz)

199.T "Understanding the Nanostructure of Al_2O_3 ALD Films on a Layered Cathode Oxide Surface Using Molecular Dynamics Simulation" · AIChE National Meeting · Phoenix, AZ · Nov 14, 2022 (by Julie Ngyen, Al Weimer, and Hendrik Heinz)

198.T "Simulation of Nanomaterials and Composites from Atoms to Micrometers in Order of Magnitude Higher Accuracy: Models, Examples, and Applications" · 10^{th} Int. Conf. on Multiscale Materials Modeling (MMM-10) · Baltimore, MD · October 5, 2022 (by Cheng Zhu and Hendrik Heinz)

197.P "CSSI Framework: Cyberloop for Accelerated Bionanomaterials Design" · NSF CSSI PI Meeting · Alexandria, VA · July 25-26, 2022 · https://zenodo.org/record/6842341

196.T "Machine Learning for Carbon Nanotube Yarn Mechanical Properties" · MRS Spring Meeting · Honolulu, HI · May 11, 2022 (by Jordan Winetrout and Hendrik Heinz)

195.P "Adsorption and Diffusion of Oxygen on Pure and Partially Oxidized Metal Surfaces" · MRS Spring Meeting · Honolulu, HI · May 11, 2022

194.P "Protein Assembly on Iron Oxide Nanoparticles for Enhanced In Vivo Delivery in HeLa Cells" · MRS Spring Meeting · Honolulu, HI · May 9, 2022

193.T "Accurate Atomistic Simulations of Metals, Oxides and Hydroxides up to the Large Nanometer Scale" · NSF Cyberloop Workshop · Virtual · Nov 18, 2021 (by Krishan Kanhaiya and Hendrik Heinz)

192.T "Interface Force Field for sp3 Diamond Crystal Structures: Regression-Driven Development" · AIChE Fall Meeting · Boston, MA · Nov 11, 2021 (by Katarina Odak, Al Weimer, and Hendrik Heinz)

191.P "Si and C Models as the Basis for Regression-Driven Development of the Interface Force Field" · AIChE Fall Meeting · Boston, MA · Nov 9, 2021 (by Katarina Odak, Al Weimer, and Hendrik Heinz)

190.P "Simulation of the Interface between Low Cycles of ALD Films and NMC Cathode Materials Using Molecular Dynamics" · AIChE Fall Meeting · Boston, MA · Nov 8, 2021 (by Julie Ngyen, Al Weimer, and Hendrik Heinz)

189.T "Investigating Li-Ion Behavior in ALD Coated NMC Cathode Materials Via Molecular Dynamics" · AIChE Fall Meeting · Boston, MA · Nov 8, 2021 (by Julie Ngyen, Al Weimer, and Hendrik Heinz)

188.T "Machine Learning for CNT-Yarn Nanostructure Mechanical Properties" · NASA US-COMP Workshop · Online · Oct 14, 2021 (by Jordan Winetrout and Hendrik Heinz)

187.T "Prediction of Carbon Nanostructure Mechanical Properties and Role of Defects Using Machine Learning" · Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology (MMLDT-CSET 2021) · San Diego, CA, and Online · Sep 26-29, 2021 (by Jordan Winetrout and Hendrik Heinz)

186.T "Reactive Interface Force Field Development: Validation and Applications for Composites" · NASA US-COMP Workshop · Online · May 17, 2021 (by Jordan Winetrout and Sagar Patil)

185.T „Accurate Molecular Models for MoS2 and Battery Oxides (NMC) to Predict Interfacial Properties up to the Large Nanometer Scale “ · MRS Spring and Fall Meeting (online) · Nov 29 - Dec 3, 2020

184.T „Understanding CNT/Polymer Interphase Assembly and Mechanical Strength Using Simulation and Machine Learning“ · MRS Spring and Fall Meeting (online) · Nov 29 - Dec 3, 2020

183.T „Reactive Interface Force Field Development and Validation for Composites“ · NASA US-COMP Workshop (online) · Oct 7, 2020

182.T „Molecular Recognition and Assembly of Biomaterials: Computational and Data Science Tools for Property Predictions“ · TMS National Meeting · San Diego, CA · Feb 26, 2020

181.P „Cyberloop for Bionanomaterials Design“ · NSF CSSI PI Meeting · Seattle, WA · Feb 13, 2020

180.T „Cyberloop for Bionanomaterials Design“ · Cyberloop Kickoff Workshop · Organizer & Talk · CU Boulder · Oct 16 & 17, 2019

179.T „A Calcium-Silicate-Hydrate (C-S-H) Builder and Interface Modeling Tools for Full Electrolyte Simulations“ · ACerS/GFMET-2 · Toronto, Canada · Jul 25, 2019

178.T „Reactive Simulations of CNTs, Graphitic Materials, and Polymers“ · NASA STRI Meeting · Salt Lake City, UT · May 7, 2019

177.T „Insights into PMMA/CNT Assembly and Nanoscale Structure-Property Relationships in Polymer/CNT Composites“ · ACS Spring Meeting · Orlando, FL · Apr 3, 2019

176.T „Predictive Modeling of Bionanomaterials from Picometers to Micrometers“ · TMS Meeting · San Antonio, TX · Mar 12, 2019

175.T „Understanding the Impact of Ligand Composition on Protein Corona Formation around Au Nanoparticles“ · MRS Fall Meeting · Boston, MA · Nov 30, 2018 (by Samuel Hoff)

174.P „Understanding the Mechanism of Metal Oxidation on the Nanoscale—Vacancy Transport, Energy Barriers and Rate Predictions“ · MRS Fall Meeting · Boston, MA · Nov 29, 2018 (by Krishan Kanhaiya)

173.T „Barrier-Free Nucleation of 2D Phage-Selected Peptide Films on MoS2 Surfaces“ · MRS Fall Meeting · Boston, MA · Nov 29, 2018 (by Jianjun Chen)

172.T „Determining the Binding Mechanisms of All 20 Natural Amino Acids to (hkl) Facets of Hydroxyapatite as a Function of pH“ · MRS Fall Meeting · Boston, MA · Nov 26, 2018 (by Samuel Hoff)

171.T „An Accurate Force Field for Graphitic Materials Including Virtual Pi Electrons and Applications to Understand Carbon Nanotube Dispersion in Solvents and Polymer Solutions“ · AIChE Annual Meeting · Pittsburgh, PA · Nov 2, 2018 (by Michael Nathanson)

170.T „Adsorption and Reaction of Furfuryl Alcohol on Pt(111): A Comparison Study to Pd(111)“ · AIChE Annual Meeting · Pittsburgh, PA · Nov 2, 2018 (by Lesli Mark and Will Medlin)

169.T „Understanding the Mechanism of Aqueous Metal Oxidation on the Nanoscale: Vacancy Transport, Energy Barriers, and Rate Predictions“ · AIChE Annual Meeting · Pittsburgh, PA · Nov 1, 2018 (by Michael Nathanson)

168.T „Interaction of Furan and Benzene Derivatives with Palladium Nanoparticle Catalysts and the Mechanism of Conversion into Biofuels“ · AIChE Annual Meeting · Pittsburgh, PA · Nov 1, 2018 (by Lesli Mark)

167.P „Atomic-Level Insight into Oxygen Adsorption on (hkl) Platinum Surfaces and Implications for the Reactivity in the Oxygen Reduction Reaction“ · AIChE Annual Meeting · Pittsburgh, PA · Oct 31, 2018 (by Shiyi Wang)

166.T „Design of Biomaterials By Simulation and Experiment:Molecular Recognition, Assembly, and Applications“ · AIChE Annual Meeting · Pittsburgh, PA · Oct 31, 2018

165.T „Accurate Simulation of Oxides and Hydroxides up to the Large Nanometer Scale“ · AIChE Annual Meeting · Pittsburgh, PA · Oct 31, 2018 (by Michael Nathanson)

164.P „Force Field for Molybdenum Disulfide to Compute Bulk and Interfacial Properties with Electrolytes and Biomacromolecules in High Accuracy“ · AIChE Annual Meeting · Pittsburgh, PA · Oct 29, 2018 (by Juan Liu and Jin Zeng)

163.P „Mechanism of Osteocalcin Interactions with Hydroxyapatite Surfaces and Hydrogen Phosphate Precursors for Bone Mineralization“ · AIChE Annual Meeting · Pittsburgh, PA · Oct 29, 2018 (by Juan Liu and Mahdi Tavakol)

162.P „Molecular Interaction of DNA with Cysteamine- and PolylysineAcetate Modified Gold Surfaces for Single Nucleobase Identification“ · AIChE Annual Meeting · Pittsburgh, PA · Oct 29, 2018 (by Lesli Mark)

161.P „Peptide Adsorption on Hydroxyapatite Surfaces and Implications on Shape and Mineralization: Impact of Sequence and Electrolyte pH“ · AIChE Annual Meeting · Pittsburgh, PA · Oct 29, 2018 (by Juan Liu)

160.P „Simple and Accurate Method to Calculate Circular Dichroism Spectra of Peptides and Proteins in Molecular Dynamics Simulations“ · AIChE Annual Meeting · Pittsburgh, PA · Oct 29, 2018 (by Juan Liu and Zewei Wang)

159.T „Nanoscale Structure-Property Relationships of Polyacrylonitrile/CNT Composites As a Function of Polymer Crystallinity and CNT Diameter“ · AIChE Annual Meeting · Pittsburgh, PA · Oct 29, 2018

158.T „Atomic Structure and Stress Release Mechanism of Core-Shell Au-Pd Nanocubes“ · AIChE Annual Meeting · Pittsburgh, PA · Oct 29, 2018 (by M. Nathanson)

157.T „Force Field Parameters for Hydrogen, Oxygen, and Nitrogen to Study Complex Phase Equilibria and Interfacial Reactions“ · AIChE Annual Meeting · Pittsburgh, PA · Oct 28, 2018 (by S. Wang)

156.T „Amorphous Carbon Modeling“ · NASA STRI Institute Meeting · MIT, MA · Oct 25, 2018 (by M. Nathanson)

155.T „Accurate Simulation of Oxides and Hydroxides Up to the Large Nanometer Scale“ · MS&T National Meeting · Columbus, OH · Oct 18, 2018 (by K. Kanhaiya)

154.T „Carbon Nanotube Dispersion in Solvents and Polymer Solutions: Mechanisms, Assembly, and Preferences“ · MS&T National Meeting · Columbus, OH · Oct 18, 2018

153.T „Discovery of Biomaterials by Simulation and Experiment: Molecular Recognition, Assembly, Applications“ · MS&T National Meeting · Columbus, OH · Oct 17, 2018

152.P „Understanding the Mechanism of Metal Oxidation on the Nanoscale: Vacancy Transport, Energy Barriers, and Rate Prediction“ · MS&T National Meeting · Columbus, OH · Oct 16, 2018 (by K. Kanhaiya)

151.T „Adsorption and Diffusion of Oxygen on Pure and Partially Oxidized Al and Ni Surfaces“ · MS&T National Meeting · Columbus, OH · Oct 16, 2018 (by K. Kanhaiya)

150.P „Nanoscale Structure-Property Relationships of Polyacrylonitrile/CNT Composites as a Function of Polymer Crystallinity and CNT Diameter“ · ACS Fall Meeting · Boston, MA · Aug 22, 2018 (by J. Gissinger)

149.T „Discovery of Biomaterials by Simulation and Experiment: Molecular Recognition, Assembly, Applications“ · ACS Fall Meeting · Boston, MA · Aug 22, 2018

148.T „Interaction of Furan and Benzene Derivatives with Palladium Nanoparticle Catalysts and the Mechanism of Conversion into Biofuels“ · ACS Fall Meeting · Boston, MA · Aug 21, 2018

147.P „Atomic-Level Insight Into Oxygen Adsorption on (hkl) Platinum Surfaces and Implications for the Reactivity in the Oxygen Reduction Reaction“ · ACS Fall Meeting · Boston, MA · Aug 20, 2018 (by Shiyi Wang)

146.T „Peptide Adsorption on Hydroxyapatite Surfaces and Implications on Shape and Mineralization: Impact of Sequence and Electrolyte pH“ · ACS Fall Meeting · Boston, MA · Aug 20, 2018 (by Juan Liu)

145.P „Mechanism of Osteocalcin Interactions with Hydroxyapatite Surfaces and Hydrogen Phosphate Precursors for Bone Mineralization“ · ACS Fall Meeting · Boston, MA · Aug 19, 2018 (by Mahdi Tavakol and Sam Hoff)

144.T „Carbon Nanotube Dispersion in Solvents and Polymer Solutions: Mechanisms, Assembly, and Preferences“ · ACS Fall Meeting · Boston, MA · Aug 19, 2018

143.T „Long Range Hierarchical Assembly of Pt Nanocrystals – Insights from Measurements and Molecular Simulations of Nanoparticle Docking“ · ACS Fall Meeting · Boston, MA · Aug 19, 2018 (by Shiyi Wang)

142.T „IFF Development and Testing“ · NASA STRI Meeting · Tallahassee, FL · May 30, 2018

141.T „Development and Validation of Polarized Models for Graphitic Biosensors“ · AVS Meeting · Tampa, FL · Oct 31, 2017 (by Amanda Garley)

140.T „Clay/Water Interfacial Models (Kaolinite, Micas, Montmorillonite) to Reproduce Hydration Energies, Contact Angles, and Organic Adsorption“ · 16th Int. Clay Conf. · Granada, Spain · July 18, 2017

139.T „Tricalcium Silicate Hydration in Absence and Presence of Aluminate Ions: A Step Towards a Molecular Understanding of How the Hydration Rate of Cement Depends On its Formulation“ · ACS Spring Meeting · San Francisco, CA · Apr 5, 2017 (by Jean-Baptiste d’Espinose de Lacaillerie)

138.T “Reliable Computational Design of Biological-Inorganic Materials to the Large Nanometer Scale Using INTERFACE-FF” · Dechema ProcessNet · Frankfurt, Germany · Mar 10, 2017

137.T “Simulation of Biological and Nanostructured Interfaces to Discover New Materials” · AIChE Annual Meeting · San Francisco, CA · Nov 17, 2016

136.P “Diffusion of Molecular Oxygen on Low Index Ni and Al Surfaces” · MURI Review, University of Virginia · Charlottesville, VA · Jun 29, 2016 (by Krishan Kanhaiya)

135.P “Electronically Refined Force Fields for BCC and HCP Metals” · MURI Review, University of Virginia · Charlottesville, VA · Jun 29, 2016 (by Chamila Dharmawardhana)

134.P "Modeling of Mo_3Si (A15) Oxidation and Resulting Silica Morphology" · MURI Review, University of Virginia · Charlottesville, VA · Jun 29, 2016 (by Chamila Dharmawardhana)

133.P "$MoSi_2$ Oxidation: Mechanism and Silica Growth" · MURI Review, University of Virginia · Charlottesville, VA · Jun 29, 2016 (by Chamila Dharmawardhana)

132.P "Refined Parameters for Cations and Anions in Aqueous Solution for Atomistic Force Fields" · 5th World Congress on Mater. Sci. & Engr · Alicante, Spain · Jun 13-15, 2016 (by Tariq Jamil)

131.T "Mechanism of Molecular Interaction of Superplasticizer Oligomers with Hydrated Cement Phases" · 5th World Congress on Mater. Sci. & Engr · Alicante, Spain · Jun 13-15, 2016 (by Tariq Jamil)

130.T "Development of Atomistic Force Field and Interfacial Study of Cementitious Minerals" · 4th International Workshop on Mechanisms and Modelling of Waste/Cement Interactions · Murten, Switzerland · May 22-25, 2016 (by Ratan Mishra)

129.T "Tuning Catalytic Properties of Pd Nanoparticles through Bioinspired Synthesis and Control of Surface Disorder" · CU Boulder Catalysis Group · Boulder, CO · Apr 1, 2016

128.P "Development and Validation of Polarized Models for Peptide-Graphene Interactions" · APS March Meeting · Baltimore, MD · March 17, 2016 (by Amanda Garley)

127.T "Investigating the Binding of Peptides to Graphene Surfaces for Biosensing Applications" · APS March Meeting · Baltimore, MD · March 14, 2016 (by Amanda Garley)

126.P "Design and Testing of Nanoalloy Catalysts in 3D Resolution" · DoE/NSF Materials Genome Principal Investigators Meeting · Bethesda, MD · Jan 11/12, 2016 (by Yu Huang)

125.T "Development of Empirical Force Fields Parameters for Graphene/Graphite and Its Application to Biorecognition at Molecular Interface" · MRS Fall Meeting · Boston, MA · Dec 4, 2015 (by Nabanita Saikia)

123.T "Biomolecules at Gold-Water Interfaces: The Role of the Metal Polarization" · MRS Fall Meeting · Boston, MA · Dec 2, 2015 (by Marialore Sulpizi)

122.T "Modeling of High Temperature Oxidation of Ni-Cr-Al at the 1 to 100 nm Scale" · MS&T 2015 · Columbus, Ohio · Oct 8, 2015

121.T "Refined Parameters for Cations and Anions in Aqueous Solution for Atomistic Force Fields" · MS&T 2015 · Columbus, Ohio · Oct 7, 2015 (by Tariq Jamil)

120.T "Development of Accurate, Polarizable, and Transferable Force Field Parameters for Graphite and Graphene to Simulate Bionanointerfaces" · MS&T 2015 · Columbus, Ohio · Oct 7, 2015 (by Nabanita Saikia)

119.P "Mechanism of Molecular Interaction of Superplasticizer Oligomers with Hydrated Cement Phases" · MS&T 2015 · Columbus, Ohio · Oct 6, 2015 (by Tariq Jamil)

118.P "Mechanism of Molecular Interaction of Superplasticizer Oligomers with Hydrated Cement Phases" · POLYCHAR23 · University of Nebraska, Lincoln · Lincoln, NE · May 13, 2015 (by Tariq Jamil)

117.T "Towards Molecular-Level Insight into Reversible Swelling of Layered Titanates" · MRS Spring Meeting · San Francisco, CA · Apr 9, 2015

116.T "The INTERFACE Force Field to Unite Materials and Biomolecular Simulation in a Single Platform: Examples of Protein Recognition on Metals, Silicates, and Phosphates" · MRS Spring Meeting · San Francisco, CA · Apr 8, 2015

115.T "Peptide-Based Strategies to Control the Structure/Function Relationship of Nanocatalysts" · MRS Spring Meeting · San Francisco, CA · Apr 7, 2015 (by Marc Knecht)

114.P "Design and Testing of Nanoalloy Catalysts in 3D Resolution" · DoE/NSF Materials Genome Principal Investigators Meeting · Bethesda, MD · Jan 12, 2015

113.T "Molecular Interaction of Peptides and Ionic Liquids with Gold Surfaces and the Mechanism of Nanorod Growth" · MRS Fall Meeting · Boston, MA · Dec 3, 2014

112.T "Elucidation of Structure/Function Relationships of Metal Nanoparticles Using a Combination of X-Ray Diffraction, Reverse Monte Carlo, and Molecular Dynamics" · MRS Fall Meeting · Boston, MA · Dec 2, 2014

111.P "A Simple Polarizable Model for the Simulation of FCC Metals at Biological Interfaces" · MRS Fall Meeting · Boston, MA · Dec 1, 2014 (by H. Ramezani-Dakhel)

110.P "Interfacial Structure of Substituted Poly(phenyleneethynylene)s in Contact with Ligand-Stabilized CdS Nanoparticles" · MRS Fall Meeting · Boston, MA · Dec 1, 2014

109.T "A Silica Surface Model Database and Computational Prediction of Specific Peptide Binding as a Function of pH and Particle Size" · MRS Fall Meeting · Boston, MA · Dec 1, 2014

108.T "The INTERFACE Approach toward Accurate Force Field Parameters – Example Predictions for Aluminosilicates at the 1 to 100 nm Scale" · MS&T 2014 · Pittsburgh, PA · Oct 16, 2014

107.T "Nanocoatings on Clay and Cement: Understanding the Action of Surfactants and Grinding Aids" · MS&T 2014 · Pittsburgh, PA · Oct 15, 2014 (by T. Jamil)

106.T "Unraveling Molecular Mechanism of Pt{100} Recognition and Formation of Cubic Nanoparticles in Peptide Directed Synthesis" · MS&T 2014 · Pittsburgh, PA · Oct 15, 2014 (by H. Ramezani-Dakhel)

105.T "Accurate Atomistic Models of pH Responsive Surfaces of Silica and Apatite to Quantify Recognition of Proteins and Drugs" · MS&T 2014 · Pittsburgh, PA · Oct 15, 2014

104.T "Facet-Specific Molecular Recognition Mechanisms on Metal Surfaces and Applications to Nanostructure Shape Control" · MS&T 2014 · Pittsburgh, PA · Oct 15, 2014

103.T "Molecular Mechanisms of Size Control and Catalytic Functionality of Peptide-Directed Palladium Nanocrystals in Aqueous Solution" · MS&T 2014 · Pittsburgh, PA · Oct 13, 2014 (by H. Ramezani-Dakhel)

102.T "Atomic-Level Insight into Interactions of Poly(phenyleneethynylene)s with Ligand-Stabilized CdS Nanoparticles" · MS&T 2014 · Pittsburgh, PA · Oct 13, 2014

101.P "Properties of PAN-Carbon Nanotube Composites via Multiscale Simulation" · DARPA Carbon Nanofiber Review · Georgia Inst of Technology, Atlanta, GA · Oct 9, 2014 (by Jake Gissinger)

100.T "Alloys and Oxide Phases in Chemical Resolution up to the 100 Nanometer Scale: Modeling and Experiment" · MURI Kickoff Meeting on Corrosion in 4D · Evanston, IL · Oct 2, 2014

99.T "Multi-Modelling Approach to Clinker Grinding" · 34th Cement and Concrete Science Conference · Sheffield, UK · Sep 14-17, 2014 (given by Robert Flatt)

98.T "Accurate Atomistic Force Fields and Models for Cement Minerals and Aqueous Organic Interfaces" · American Ceramic Society, Cement Division Meeting (ACerS-D) · Cookville, TN · July 11, 2014

97.T "Multi-Modelling Approach to Study the Effectiveness of Grinding Aids" · American Ceramic Society, Cement Division Meeting (ACerS-D) · Cookville, TN · July 10, 2014 (with R. J. Flatt)

96.P "Atomic-Scale Examination of Bio-Derived Nanoparticles: From Structure to Catalytic Functionality" · NSF Workshop on Transformative Technologies in Molecular Simulation · University of Wisconsin, Madison, WI · May 20, 2014 (by H. Ramezani-Dakhel)

95.P "Polarizable Force Field for the Simulation of Face-Centered Cubic Metals and Biological Interfaces" · ACS Spring Meeting · Dallas, TX · Mar 18, 2014 (by H. Ramezani-Dakhel)

94.T "Mechanism of Selective Recognition of Cubic Platinum Nanocrystals by Peptides in Aqueous Solution" · ACS Spring Meeting · Dallas, TX · Mar 16, 2014 (by H. Ramezani-Dakhel)

93.T "Structure, Dynamics, and Cohesion of Clay Intercalation Compounds with Functional Surfactants" · MRS Fall Meeting · Boston, MA · Dec 4, 2013

92.T "Understanding Molecular Mechanisms of Size Control of Peptide Directed Palladium Nanocrystals and Catalytic Activity in Coupling Reactions" · MRS Fall Meeting · Boston, MA · Dec 4, 2013 (by H. Ramezani-Dakhel)

91.P "Platinum Cubic Nanocrystals: Unraveling Molecular Mechanism of Shape Control in Peptide Mediated Synthesis" · MRS Fall Meeting · Boston, MA · Dec 2, 2013 (by H. Ramezani-Dakhel)

90.T "Clay Minerals and Cement Minerals: Molecular and Interfacial Properties in Model and Experiment" Clay Minerals Society Annual Meeting · Urbana-Champaign, IN · Oct 7, 2013

89.T "Nanoscale Interfaces of Tricalcium Silicate and Organic Dispersants in Cement – Agglomeration and Initial Hydration" · ACS National Meeting (D-COLL) · Indianapolis, IN · Sep 11, 2013

88.T "Understanding Molecular Recognition and Growth of Nanostructures from a Molecular Perspective" · Workshop Directed Assembly of Functional Nanomaterials · University of Strathclyde, Glasgow, UK · June 13, 2013

87.T "Understanding the Effectiveness of Polycarboxylates as Grinding Aids" · 10th Int. Conference on Superplasticizers and Other Chemical Admixtures in Concrete · Prague, Czech Republic · October 29, 2012 (by R. K. Mishra)

86.T "Control Over Self Assembly of Diblock Copolymers on Hexagonal and Square Templates for High Area Density Circuit Boards" · ACS Fall Meeting (D-POLY) · Philadelphia, PA · Aug 24, 2012

85.T "Influence of the Shape of Nanostructured Metal Surfaces on Adsorption of Singel Peptide Molecules in Aqueous Solution" · ACS Fall Meeting (D-POLY) · Philadelphia, PA · Aug 22, 2012

84.T "Stabilization Mechanism of Cubic Platinum Nanocrystals in Peptide Mediated Synthesis" · ACS Fall Meeting (D-POLY) · Philadelphia, PA · Aug 22, 2012 (given by H. Ramezani-Dakhel)

83.P "Interaction of Substituted Poly(phenylene ethynylene) with Core-Shell CdS Nanoparticles" · ACS Fall Meeting (D-ENFL) · Philadelphia, PA · Aug 22, 2012 (given by H. Liu)

82.P "Abstraction Energy Controls Catalytic Activity of Palladium Nanocrystals in Atom Leaching Carbon-Carbon Coupling Reactions" · ACS Fall Meeting (D-COMP) · Philadelphia, PA · Aug 22, 2012 (given by H. Ramezani-Dakhel)

81.P "Simulation of Dye Sensitized Solar Cells" · ACS Fall Meeting (D-POLY) · Philadelphia, PA · Aug 21, 2012 (given by H. Liu)

80.P "Towards Rational Biomimetic Design: A Dynamic Phenyl Molecular Switch for Pt {111} Facet Recognition" · ACS Fall Meeting (D-COLL) · Philadelphia, PA · Aug 21, 2012 (given by L. Ruan)

79.P "Surface Properties of Hydroxyapatite and Molecular Models for the Simulation of Hybrid Interfaces" · ACS Fall Meeting (D-COLL) · Philadelphia, PA · Aug 21, 2012 (given by T. J. Lin)

78.T "Nanomechanics and Dispersion of Layered Silicates in Polymer Matrices: Moduli, Cleavage Energy, and Free Energy of Exfoliation" · S-Polymat 2012 · Kerkrade, Netherlands · May 22, 2012

77.T "Bending of Layered Silicates on the Nanometer Scale: Mechanism, Stored Energy, and Curvature Limits" · ACS Spring Meeting (D-COLL) · San Diego, CA · Mar 29, 2012

76.T "Nanomechanics and Dispersion of Layered Silicates in Polymer Matrices: Moduli, Cleavage Energy, and Free Energy of Exfoliation" · ACS Spring Meeting (D-INOR) · San Diego, CA · Mar 29, 2012

75.T "Atomistic Simulation of Aqueous Silica Interfaces" · ACS Spring Meeting (D-INOR) · San Diego, CA · Mar 27, 2012 (given by F. S. Emami)

74.T "Cleavage Energy of Tricalcium Silicate and Interactions with Amine Additives" · 13th Int. Congress on Cement Chemistry · Madrid, Spain · Jul 7, 2011 (given by R. K. Mishra, won best short presentation award).

73.T "Molecular Understanding of Directional Surface and Interface Tensions of Gypsum and Plaster of Paris" · 13th Int. Congress on Cement Chemistry · Madrid, Spain · Jul 7, 2011 (given by R. K. Mishra).

72.P "Nanomechanics, Bending Stability, and Failure of Layered Silicates as Function of CEC and Stress" · MRS Fall Meeting · Boston, MA · Dec 2, 2010

71.T "Molecular Mechanism of Peptide Binding to Silica Surfaces − Experiment and Simulation" · MRS Fall Meeting · Boston, MA · Dec 1, 2010

70.T **"**Tuning Exfoliation Thermodynamics by Surface Modification of Organoclays**"** · PPS-26 Istanbul · Istanbul, Turkey · Oct 20, 2010

69.T "Molecular Models and Methods to Understand Self-Assembly of Inorganic-Bioorganic Multiphase Materials" · ACS Fall Meeting 2010 · Boston, MA · Aug 26, 2010

68.T "An Accurate Force Field and Atomistic Models for Tricalcium Silicate, Alite, and Adsorption of Molecular Grinding Aids" · NIST Computer Modeling Workshop · Gaithersburg, MD · Aug 11-13, 2010 (given by R. Mishra)

67.T "Molecular Mechanisms of Selective Peptide-Metal Interactions and Effects on Particle Growth" · OCCBIO 2010 · Columbus, OH · Jun 15, 2010 (given by J. Feng)

[Further talks by R. J. Berry, R. B. Pandey in between not listed here]

66.T "Directed Self-assembly of Block Copolymers on Topological Substrates: A Monte Carlo Simulation" · AIChE Meeting · Nashville, TN · Nov 11, 2009 (given by J. Feng)

65.T "Quantifying Adsorption of Amino Acids and Surfactants on Au {111} Surfaces in Aqueous Solution" · ACS Fall National Meeting · Washington, DC · Aug 19, 2009 (given by J. Feng)

64.T "Nature of Molecular Interactions of Peptides With Gold, Palladium, and Pd-Au Bimetal Surfaces in Aqueous Solution" · ACS Fall National Meeting · Washington, DC · Aug 17, 2009

63.T "Accurate Simulation of Layered Silicates and Their Interfaces" · 14th Int. Clay Conf. · Castellaneta Marina, Italy · Jun 18, 2009

62.T "Structure and Cleavage Energy of Surfactant-Modified Clays: Influence of CEC, Head Group, and Chain Length" · 14th Int. Clay Conf. · Castellaneta Marina, Italy · Jun 14, 2009

61.P "Trends in Cleavage Energies of Alkylammonium-Modified Layered Silicates as a Function of Cation Density, Head Group Structure, and Chain Length" · Y. T. Fu, HH et al. · APS March Meeting · Pittsburgh, PA · Mar 16−20, 2009

60.P "Quantifying Polarization at Metal-Biological Interfaces in Solution" · K. C. Jha, HH et al. · APS March Meeting · Pittsburgh, PA · Mar 16−20, 2009

59.P "Simulation of Peptide Binding to Silica and Silica Mineralization" · F. S. Emami, HH et al. · APS March Meeting · Pittsburgh, PA · Mar 16−20, 2009

58.T "Atomistic Simulation of Cleavage Energy of C3S and Organic-silicate Interactions" · R. K. Mishra, HH et al. · NanoCem Workshop · Derio, Spain · Mar 3, 2009

57.T "Peptide Binding to Metal, Bimetal, and Layered Silicate Even Surfaces" · MRS Fall Meeting · Boston, MA · Dec 1, 2008 (given by R. B. Pandey)

56.T "Adsorption of Single Amino Acids and Surfactants to Au {111} Surfaces In Aqueous Solution - Insight from Atomistic Simulation" · AIChE Annual Meeting · Philadelphia, PA · Nov 20, 2008 (given by J. Feng)

55.T "Atomistic Simulation of Poly(ethylene oxide) In Aqueous Solution: Challenges and Suggestions for Models" · AIChE Annual Meeting · Philadelphia, PA · Nov 17, 2008 (given by J. Feng)

54.P "Design of Functional Nanoparticle-Peptide Interfaces Guided By Atomistic Simulation" · AFOSR Biotech Review · Arlington, VA · Nov 12/13, 2008 (given by R. J. Berry)

53.P G. D. Zartman & HH: "Calculation of Nanoscale Elastic, Shear, and Bending Properties of Sheet Silicates Using Molecular Dynamics Simulation" · PINO Meeting · Case Western Reserve University, OH · Jul 3, 2008

52.T "A Force Field for Layered Silicates and Simulation of Interfaces with Surfactants: Structure, Surface Energy, and Phase Transitions" · PPS-24 · Salerno, Italy · June 18, 2008

51.T "Peptide Binding to Sheet Silicate and Metal Nanoparticles: Insight from Atomistic Simulation and Experiment" · PPS-24 · Salerno, Italy · June 17, 2008

50.T Y. T. Fu & HH: "Modification of surface energies of layered silicates through surfactants of different chain length" · ACS National Meeting · New Orleans, LA · Apr 9, 2008

49.T "Peptide Binding to Sheet Silicate and Metal Nanoparticles - Insight from Atomistic Simulation" · ACS Spring Meeting · New Orleans, LA · Apr 06, 2008 (B. L. Farmer)

48.T "Photoisomerization of Azobenzene: A Quantitative Force Field-based Implementation and Simulation of Assemblies with Layered Silicates in Comparison with Experiment" · ACS Spring Meeting · New Orleans, LA · Apr 06, 2008

47.T "Relation between Packing Density and Thermal Transitions of Alkyl Chains on Layered Silicate and Metal Surfaces" · MRS Spring Meeting · San Francisco, CA · Mar 27, 2008

46.P G. D. Zartman & HH: "Calculation of Nanoscale Elastic, Shear, and Bending Properties of Sheet Silicates Using Molecular Dynamics Simulation" · MRS Spring Meeting · San Francisco, CA · Mar 27, 2008

45.P K. C. Jha & HH: "Polarization Effect at Peptide-Gold Interfaces Estimated by MD Simulation" · MRS Spring Meeting · San Francisco, CA · Mar 26, 2008

44.T "Peptide Binding to Sheet Silicate and Metal Nanoparticles - Insight from Atomistic Simulation" · MRS Spring Meeting · San Francisco, CA · Mar 25, 2008

43.P "Relation between Packing Density and Thermal Transitions of Alkyl Chains on Layered Silicate and Metal Surfaces" · APS March Meeting · New Orleans, LA · Mar 12, 2008

42.T "Peptide Binding to Sheet Silicate and Metal Nanoparticles: Insight from Atomistic Simulation" · APS March Meeting · New Orleans, LA · Mar 10, 2008 (R. B. Pandey)

41.P "Atomistic Simulation of Inorganic-Biological Interfaces and Accurate Force Fields for FCC Metals and Layered Silicates" · Zing Conference on Computational Biophysics with Chemical Accuracy · Jolly Beach Resort · Bolans Village, Antigua · Jan 15, 2008

40.T "Self-Assembly of Peptides on Montmorillonite Nanoparticles" · AIChE Annual Meeting · Salt Lake City, UT · Nov 7, 2007

39.T "Atomistic Simulation of Peptide Binding to Metal Nanonoparticle Surfaces" · AIChE Annual Meeting · Salt Lake City, UT · Nov 6, 2007

38.T G. D. Zartman & HH: "Nanomechanics of Sheet Silicates" · NASA Glenn Undergraduate Conference · Cleveland, OH · Aug 8, 2007

37.T "Atomistic Simulation of the Interaction of Peptides with Metal and Sheet Silicate Nanoparticles" · Mainz Materials Simulation Days 2007 · Max-Plack-Institute for Polymer Research · Mainz, Germany · June 13, 2007

36.T "Force Fields for Sheet Silicates and Metals" · AIChE Annual Meeting · San Francisco, CA · Nov 17, 2006

35.T "Calculation of Local Pressure Tensors in Systems with Many-Body Interactions" · AIChE Annual Meeting · San Francisco, CA · Nov 17, 2006

34.T "Simulation of Interfaces in Nanocomposites and Biomaterials" · University of Akron Sponsor's Day Dept of Polymer Eng · Akron, OH · Oct 26, 2006.

33.T "Force Fields for Inorganic Components in Hybrid Systems" · ACS National Meeting San Francisco · Sep 13, 2006

32.T "Simulation of Peptide Binding to Metal and Clay Nanoparticles" · AFRL/MLBP WPAFB · OH, Aug 22, 2006.

31.P "Simulation of Polymer Adsorption on Surfaces" · Gordon Research Conference on Polymer Physics · Connecticut College, CT · Jul 23-28, 2006

30.P "Atomistic Simulation of Organic-Inorganic Interfaces Containing Sheet Silicates" · ACS Dayton section · Annual Poster Session · Dayton, OH · Mar 7, 2006

29.T ”Towards Quantitative Modeling of Surface Properties in Inorganic-Organic Hybrid Materials” · AFRL–Sandia National Laboratory Collaborative Meeting · WPAFB · November 8, 2005

28.T “Calculation of Local Pressures in Systems with Many-Body Interactions” · Rutgers University, NJ · Department of Applied Mathematics · 93rd Statistical Mechanics Conference · May 16, 2005

27.T ”Computer Simulation of the Light-Induced Trans-Cis Isomerization of Azobenzene Grafted Onto Montmorillonite Sheets” · MRS Fall Meeting · Boston, MA · Nov 31, 2005

26.P “Modeling of the Photochemical Trans-Cis Isomerization of Azobenzene Confined Between Montmorillonite Sheets” · MRS Fall Meeting · Boston, MA · Nov 31, 2005

25.P “Towards Quantitative Modeling of Interface Properties of Organic-Inorganic Hybrid Materials” · AIChE Annual Meeting · Cincinnati, OH · Oct 31, 2005

24.T "Calculation of Local Pressure Tensors in Systems with Many-Body Interactions" · ACS national meeting · Washington, D. C. · Sep 1, 2005

23.T "Free Energy of Exfoliation Between Layered Silicate Sheets" · ACS national meeting · Washington, D. C. · Aug 31, 2005

22.T "Towards Quantitative Modeling of Surface Properties in Inorganic-Organic Hybrid Materials" · ACS national meeting · Washington, D. C. · Aug 31, 2005

21.P “Towards Quantitative Modeling of Interface Properties of Organic-Inorganic Hybrid Materials” · ACS National Meeting (AEI) · Washington, D. C. · Aug 29, 2005

20.T "Self-Assembly of Alkylammonium Chains on Montmorillonite: Effect of Chain Length, Head Group Structure, and Cation Exchange Capacity" · ACS national meeting Washington, D. C. · Aug 28, 2005

19.P “Free Energy of Exfoliation Between Layered Silicate Sheets” · Symposium “Oligomers to Macromolecules in Akron” · University of Akron, OH · Jun 27, 2005 · With R. A. Vaia and B. L. Farmer

18.T “Progress in Molecular Modeling of Superplasticizers in Cementitous Systems” · ETH Zurich · Department of Materials · Apr 14, 2005

17.P “Conformation and Dynamics of a Flexible Sheet in Solvent Media by Monte Carlo Simulations” · APS March Meeting · Los Angeles, USA · Mar 21-25, 2005 · By Pandey, R.; Anderson, K. L.; Heinz, H.; Farmer, B.

16.T “Atomic Charges for Classical Simulations of Polar Systems” · WATOC 2005—7th World Congress of Theoretically Oriented Chemists · Cape Town, South Africa · Jan 19, 2005

15.T “Semiempirical Atomistic Simulation of Interactions between Sheets of Layered Silicates” · MRS Fall meeting · Boston, MA · Dec 1, 2004

14.T “A Semiempirical Energy Model and Atomistic Simulation of Organically Modified Montmorillonite” · MRS Fall meeting · Boston, MA · Dec 1, 2004

13.T “A Semiempirical Energy Model and Atomistic Simulation of Organically Modified Montmorillonite” · AFRL/ML · Polymer Technology Colloquium · Wright-Patterson AFB Dayton, OH · Nov 24, 2004

12.T “Structure and Phase Transitions of Alkylammonium Chains on Mica” · ACS national meeting · Philadelphia, PA · Aug 26, 2004

11.P "Atomic Charges for Classical Simulation of Polar Systems” · ACS national meeting · Philadelphia, PA · Aug 23, 2004 · With U. W. Suter

10.P "Atomistic Modeling of Organically Modified Mica" · NANO 2004 · Wiesbaden, Germany · Jun 22-26, 2004 · With U. W. Suter

9.T "Atomic Charges for Classical Simulations of Polar Systems" · APS march meeting · Montreal, Canada · Mar 26, 2004

8.T "A Perylene Chromophore in *n*-Alkanes: Modeling Geometries and $\pi \rightarrow \pi^*$ Spectral Shifts Based on Local Electron Density" · APS march meeting · Montreal, Canada · Mar 26, 2004

7.P "Atomistic Modeling of Organically Modified Mica" · 20th Annual Meeting of the Swiss User Group Surfaces and Interfaces · Fribourg, Switzerland · Jan 23, 2004 · With U. W. Suter

6.T "Molecular Modeling of Superplasticizers in Cementitious Systems: Introductory Steps" Sika Technology AG · Zürich, Switzerland · Jan 22, 2004

5.T "Understanding Materials by Atomistic Simulation?" · Annual Meeting of the Association for the International Chemistry Olympiad · University of Leipzig, Germany · Jan 8, 2004

4.P "Structure and Phase Transitions of Alkyl Chains on Mica: Understanding by MD Simulation" · NATO-Advanced Study Institute "Computer Simulation of Surfaces and Interfaces" · Albena Black Sea Resort · Albena, Bulgaria · Sep 9-20, 2002 · with H. J. Castelijns and U. W. Suter

3.P "Partial Charges in Polar Solids" · 6th World Congress of Theoretically Oriented Chemists (WATOC) · Lugano, Switzerland · Palazzo dei Congressi · Aug 4-9, 2002 With U. W. Suter

2.T "Dynamics of Alkane Chains on Mica" · ETH Zurich · Department of Materials · Materials Science Seminar · Jul 3, 2002

1.P "MD-Simulation of Phase Transitions in Alkyl-Layered Mica Particles" · Center Stefano Franscini Monte Verità · Ascona, Switzerland · Workshop on Atomistic to Continuum Models for Long Molecules and Thin Films · Jul 15-20, 2001 · with U. W. Suter

---

Teaching Experience

Classes Taught

Type	Credits	Title	Avg Size	Code	Dates
U Colorado Boulder					
BS/PhD	3	Polymer Engineering	25	CHEN 4460/5460	Fall 2024, 2025
BS	3	Chemical Engineering Materials	50	CHEN 4440	Spring 2017-2026
BS	3	Senior Chemical Engineering Laboratory	35	CHEN 4130	Fall 2016-2021
BS	3	Fluid Mechanics	100	CHEN 3200	Spring 2016

MS	3	Intermediate Chemical Engineering Thermodynamics	35	CHEN 5370	Fall 2015
U Akron					
MS	3	Simulation of Nanoscale Materials	7	9841:777	Fall 2010, 2012
MS	3	Advanced Functional Polymers	10	9841:778	Fall 2007, 2009
MS	3	Polymer Nanocomposites (team-taught)	6	9841:770	Spring 2008
MS	3	Advanced Characterization of Functional Polymers	11	9841:715	Fall 2008, 2011
MS	2	Multiscale Simulation of Materials	10	9841:797	Spring 2007
BS	3	Engineering Properties of Polymers	10	9841:450	Spring 2008-2014
MS/ BS	1	Department Seminar (Organizer)	60	9841:601	Spring 2007

- Assistant Lab Supervisor · ETH *Zurich* · Switzerland 02/2003 − 03/2003
  Undergraduate lab course in polymer science (with Peter Walde)
- Tutoring 2001 − 2003
  Taught several undergraduate students in chemistry, physics, and mathematics
- Lecturer · Student Association ETH Zurich 07/2000
  Taught a daily thermodynamics class for 4 weeks with problem sets to prepare 1st and 2nd year undergraduates for exams (1st and 2nd year)
- Teaching Assistant · ETH Zurich 04/2000 − 07/2000
  Assisted an undergraduate class in environmental chemistry (with U. Mueller-Herold)
- Teaching Assistant · Leibniz-Institute for Education in the Natural Sciences 1995 − 1998 Germany
  Prepared selected high school students for the International Chemistry Olympiad (4 preparatory spring and summer schools, developed problem sets for qualifying exams, supervised lab courses) · University of Kiel and Ministry of Education · With Wolfgang Buender and Wolfgang Hampe

Media produced for class use:

At CU Boulder (2015-present):

- New lecture notes, homework, and class demonstrations for Chemical Engineering Materials CHEN 4440, clicker questions, and e-quizzes
- Revisions of experiment descriptions and report templates for the Senior Undergraduate Chemical Engineering Laboratory CHEN 4130, including Aspen and COMSOL simulations
- Lecture notes and revised homework assignments for Intermediate Chemical Engineering Thermodynamics CHEN 5370 (27 lectures)

At U Akron (2012-2015)

- Designed lecture notes and homework for Engineering Properties of Polymers (9841:450)
- Prepared computational workshops for interactive lectures in Simulation of Nanoscale Materials (9841:777). Equipped the computer teaching laboratory with software and demonstrations for QM/molecular simulations and materials modelling (procured, installed, and tested software including Materials Studio, VMD, NAMD on workstations with examples).

Mentoring

- **Advisor of postdocs:**

  10. Dr. Cheng Zhu, 09/2019 – 08/2023, Associate Prof. at Guangdong Technion - Israel Institute of Technology (GTIIT)
  9. Dr. Juan Liu, 07/2016 – 07/2019, Professor at Dalian Maritime University
  8. Dr. Chandrani Pramanik, 2015-2017, Tata Steel
  7. Dr. Chamila Dharmawardhana, 2016-2017, George Washington U
  6. Dr. Nabanita Saikia, 2014-2016, Assistant Professor, New Mexico Highlands University
  5. Dr. Nada Mehio, 2016, LANL
  4. Dr. Ali Javadi, 2014-2016 (co-supervised with Mark Soucek), Sherwin Williams
  3. Dr. Sanket Deshmukh, 2014-2015, Assistant Professor at Virginia Tech
  2. Dr. Jie Feng, 2008-2011, NETL Pittsburgh
  1. Dr. Pratyush Dayal, 2007-2008, IIT Gandhinagar

- **Advisor of PhD students:**

  Current:

  17. Sean Florez, 9/2024-present

      Catalysts for hydrogen storage materials

  16. Leo Beck, 10/2023-present

      Hybrid organic-inorganic structures for photovoltaics and LEDs

Graduated:

  15. Isaac Armstrong, 09/2020-12/2025, PhD Exam 12/2025

      CO_2 capture in ionic liquids and polymer structures

  14. Jordan Winetrout, PhD Exam 05/2024
      " Analysis of Composite Material Properties with the Reactive Interface Force Field and Hierarchical Spatial Graph Neural Networks”

  13. Krishan Kanhaiya, PhD exam 07/2022
      “Development and Application of Reliable Models for the Simulation of Metals and Oxides at the Nanoscale”

12. Samuel E. Hoff, PhD exam 08/2021
    "Understanding Interactions and Organization of Biological Interfaces at the Nanoscale Using Molecular Dynamics"
11. Shiyi Wang, PhD Exam 06/2021
    "Atomic-Level Understanding of Interfacial Processes on Platinum Nanostructures: From Model Developments to Applications in Catalysis"
10. Dr. Amanda Garley, PhD Exam 06/2019 (CU Boulder)
    „Nanoscale Surface Adsorption in All-Atom Resolution"
9. Dr. Tariq Jamil, PhD Exam 08/2018 (CU Boulder)
    „Understanding the Dynamics of Multiphase Cement and Clay-Based Materials from the Nanoscale"
8. Dr. Hadi Ramezani-Dakhel, PhD Exam 04/2015 (U Akron)
    "Bioengineered Metal Nanoparticles: Shape Control, Structure, and Catalytic Functionality"
7. Dr. Tzu-Jen Lin, PhD Exam 05/2013
    "Molecular Understanding of Apatite Mineralization Processes and Specific Protein Binding Using Validated Force Field Models"
6. Dr. Fateme Sadat Emami, PhD Exam 04/2013
    "Accurate Models for Silica Surfaces and Understanding Peptide Selectivity in Silica Biomineralization Processes"
5. Amir Vahid, PhD Exam 04/2012 (co-supervised with J. Richard Elliott)
    "Discontinuous Molecular Dynamics Models and Applications"
4. Dr. Hua Liu, PhD Exam 05/2013
    "Multiscale Models and Coarse-Grain Simulation of Solar Cells"
3. Dr. Ratan Kishore Mishra, PhD Exam 03/2012
    "Molecular Modeling of Polymer Interfaces in Calcium Silicates and Sulfates for Improved Cement and Wallboard Materials"
2. Dr. Yao-Tsung Fu, PhD Exam 01/2011
    "Molecular Simulation of Dispersion and Mechanical Stability of Organically Modified Layered Silicates in Polymer Matrices"
1. Dr. Kshitij Chandra Jha, PhD Exam 01/2011
    "Polarization and Self-Assembly at Metal-Organic Interfaces: Models and Molecular Level Processes"

- **Advisor of PhD Students at U Akron who remained at U Akron upon relocation to CU Boulder, changed advisor (subsequently co-advised) and completed their PhD degree**

2. Masoud Sobani, (adm. 2014); completed with Sadhan Jana at U Akron, now industry
    Rational Computational Design and Testing of Biocatalysts and Layered Materials
1. Ali Javadi, (adm. 2014); completed with Mark Soucek at U Akron, now PPG
    Understanding and molecular design of additives in cement

- **Advisor of M.S. students:**

  8. Nicolas Villoria Vasquez de Parga 08/2025-02/2026, M. S., modeling of ions (incl. MS Thesis)
  7. Barbara Morales, 12/2021-05/2023, M. S., perovskites
  6. Julie Nguyen, 07/2020-04/2023, M.S., advanced battery materials (joint with Al Weimer)
  5. Katarina Odak, 07/2020 – 12/2021, graduated with M. S., then full time Weimer lab, SiC_x phase change materials in solar thermal reactors
  4. Lesli Mark, 09/2015 – 03/2019, (co-supervised with Will Medlin), graduated with M.S., then Ph.D. study with Will Medlin
     Design of Pd Catalysts for Biofuel Conversion
  3. Michael Nathanson, 09/2016 – 08/2018, graduated with M. S., then industry (Intel)
     Molecular models and interfacial phenomena in alloys and composites
  2. Jacob R. Gissinger, 10/2014-02/2017; graduated with M. S.; then Ph.D. study with Rob Davies
     Rational Design of Carbon Nanofiber Composites
  1. Heijn J. Castelijns, at ETH Zurich, 2002

     Clay surfaces and interfaces (under direction of Prof. U. W. Suter)

- **Advisor of visiting Ph.D. students, postdocs, and professors:**

  16. Tamas Nagy, Ph. D. student at University of Debrecen (Hungary), 2020-2022, graduated 09/2022
  15. Savannah Downing, Ph. D. student, 01/2020 – 06/2020, then industry (Archerdx, Boulder)
  14. Prof. Ronald F. Ziolo, CIQA, MX, 08/2018 – 12/2018
  13. Mahdi Tavakol, PhD student at Sharif U Technology, 02/2018 – 10/2018
  12. Dr. Ratan K. Mishra, postdoc at ETH Zurich, 2012-2018
  11. Joseph R. Manning, PhD student at U Sheffield, 02/2018-07/2018, (RSC Research and Mobility Fellow)
  10. Peiying Li, PhD student at Tokyo Tech U, Japan, Spring 2017
  9. Thomas Underwood, PhD student at U Durham, UK, Spring 2016
  8. Sung-Jun Kim, Ph.D. student at U Akron, Spring 2015
  7. Masoud Sobani, (08/2014-08/2015); Ph.D. student; graduated with Sadhan Jana at U Akron after move from U Akron to U Colorado, now industry
     Rational Computational Design and Testing of Biocatalysts and Layered Materials
  6. Ali Javadi, (08/2014-08/2015); Ph.D. student, graduated with Mark Soucek at U Akron upon move to U Colorado, now industry
     Understanding and molecular design of additives in cement
  5. Prof. Han-Xue Hou, on sabbatical from Shandong U, China, 2013

4. Dr. Rajiv Berry, Air Force Research Laboratory, 2010-2015
3. Dr. Donald Wiff, Western Reserve Nano and Microsystems, 2009-2015
2. Dr. Jian-Jie Liang, Accelrys/Biovia, on sabbatical 2008
1. Leon Perez, PhD student at U Antioquia, Colombia, 2008

- **Advisor of undergraduate students (independent study, REU, senior thesis):**

39. Talal Albash, Spring 2026
38. Hassan Rabaan, Fall 2025
37. William Weise, Spring 2025
36. Roan Gerrald, Fall 2024-2025 (Senior Thesis, co-advised with Carson Bruns)
35. Paulina Apanel, Summer 2024-2025 (Senior Thesis)
34. Molham Alforidi, Spring 2024
33. William Ashcraft, Fall 2023-Spring 2024
32. Sahar Kurani, Fall 2023
31. Robert Benke, Fall 2022 and Spring 2023 (Senior Thesis)
30. Sean Oishi-Holder, Fall 2022 and Spring 2023
29. Abdulkadir Said, Summer 2022
28. Teeb Alnaji, Summer 2022
27. Lena Bokhari, Summer 2022
26. Matthew James Wong, Spring 2022
25. Abigayle Becker, Fall 2021 and Spring 2022
24. Cindy Li, Fall 2021
23. Ebrahim Alwahedi, Fall 2021
22. Ghalia Altabakh, Fall 2021
21. Omkar R. Shinde, Fall 2020
20. Daisy Fuchs, Summer 2019
19. Alfaia BaSallom, Summer 2018
18. Mohammad A. Alferayan, Summer 2018
17. Khalifah Alkhudair, Summer 2018
16. Kaiyi Hou, Summer 2018
15. Jingwen Gong, Summer 2018
14. Muhammad Azamuddin Hassan, Spring 2018
13. Victor Bader, 2017-2018

12. Darice Guittet, 2017-2018
11. Jin Zeng, all year 2017
10. Zewei Wang, all year 2017
9. Raka Ghosh-Dastidar, Summer 2017
8. Marcus Sharp, Summer 2017 (UROP)
7. Aron Jessien, Summer 2017
7. Mohammed Almarri, Summer 2017
6. Adam Cronce, Spring 2017
5. Christopher Kirby, 2016 (from Rochester Institute of Technology)
3. Gregory D. Zartman, 2007-2008, Goodyear Inc.
2. John Repasky, 2008, Sony DADC
1. Michael Heinrich (2003 at ETH Zurich)

- Placement of PhD students:
  Lawrence Berkeley National Lab, Oak Ridge National Laboratory, AFRL, NREL, U.S. patent office, postdocs (Institute Pasteur/CNRS (France), U Chicago, Georgia Tech, Northwestern U), faculty (IIT Hyderabad, Chung Yuan Christian University, Taiwan; NED University of Science and Technology, Pakistan), industry (BASF, PPG, Whirlpool), founders of start-up companies (Biena Tech)
- Placement of postdocs: faculty (Virginia Tech, Israel-Guangdong Technion – GIIT, IIT Gandhinagar, Dalian Maritime University, New Mexico Highlands University), government (NETL), industry (Tata Steel, Sherwin Williams), 2nd postdocs (George Washington U, Michigan Tech U)

Memberships and Affiliations

- Royal Society of Chemistry, fellow
- American Physical Society, member
- American Ceramic Society (ACerS), member
- American Chemical Society, member
- Materials Research Society, member
- Mineralogical Society (MinSoc), member
- TMS, member
- German Chemical Society (GDCh), member

Service

1) Service to the Department, College, and University

University of Colorado Boulder (2015-present):

- Member of CU Boulder Task Force on the Genesis mission (2026-present)

Identifying and addressing university-wide opportunities for AI-enabled scientific discovery and innovation

- Vice Chair, Faculty Governance Committee of the College of Engineering (2025-present)
  Identifying and addressing College-wide opportunities in faculty affairs and efficiency of operations based on climate and engagement surveys

- Member, Department Faculty Committee (2018-present)
  Input on departmental operations: faculty recruiting, awards nominations, mentoring, reappointment, promotion and tenure reviews, improving faculty experience

- Chair, Committee for research integrity (2023-2025)
  Evaluation and oversight in investigations in potential research misconduct in collaboration with committee members and the VP for research compliance

- Executive committee, Annual Boulder Frontiers Symposium (2019-2022)
  Leadership in planning for the annual ChBE symposium

- Member, Faculty Search Committee (2015-2018)
  Reviewed candidate files, preparing rankings and recommendations to select candidates for interviews. Hosted faculty candidates and discussed feedback.

- Member, Dissertation/Thesis Committees
  10+ internal and external PhD thesis committees (e.g., James Weltz, ChBE, Pengxiao Hao, ChBE, Mengyuan Wang, MSE, Gopal Ramalingam, U Virginia MSE, multiple international: India, Germany, etc).
- Member of 20+ Ph.D. Qualifying Exam Committees

University of Akron, Ohio (since tenure in 2012):

i) Within the Department of Polymer Engineering

- Chair, Department Visitation Committee (2014-2015)
  Organizing tours of the department and institute facilities for visitors from industry, government labs, and academia, lunches/sign up for individual meetings with faculty.
- Chair, Department Admissions Committee (2012-2014, Member, 2007-2012)
  Along with three colleagues, we reviewed candidate files and made recommendations for PhD or Master's admission, held meetings, communicated with the grad school, faculty, and departmental officer for graduate student admissions.
- Member, Department Curriculum Committee (2008-2014)
  Evaluated and contributed to changes in curriculum.
- Member, Bayer Lectureship Committee (2009-2012)
  Identifying speakers, coordination of visit
- Member, 3 PhD thesis committees during 2012-2015.
- Co-Chair, 25th Anniversary Organization Committee of DPE (2007-2008)

iii) Within the University

- Member, University Curriculum Committee (2008-2010)

- Member, Curriculum Committee of the Graduate Council (2007-2008)
- Member, Provost Advisory Committee (2008-2010)
- Member, President's Advisory Committee (2009-2011)

2) Professional societies

- Royal Society of Chemistry: Member, Newton Fellowship Committee (selects Newton postdoc fellowships)
- American Chemical Society: Member, Awards Committee of the Division of Colloid and Interface Science (selects awardees among nominations received)

3) Editor

- Senior Editor for the American Chemical Society, *Langmuir* – the ACS journal of colloids and interfaces (2021- present), IF ~4

  Evaluation of ~400 manuscripts a year through initial assessment, selection of referees and coordination of peer review (~60% overall rejection rate). Working with personal editorial assistant (ACS), editorial team, ACS staff, authors, referees. Conception of special issues, workshops, participation in editorial conferences to develop the journal. Handling rebuttals, comments, and advising in cases of ethical misconduct.

- Lead Guest editor for T&F "Molecular Simulation" for a special issue on AI in molecular simulation (2025-2026)
- Associate Editor for the Royal Society of Chemistry, New J. Chem. (2017-2021), IF ~4 at the time

  Evaluation of 300-400 manuscripts a year. Similar duties as at ACS. Working with RSC staff (located in Cambridge, UK) to address questions from authors and referees. Commissioning of perspectives and focus articles, advising in cases of ethical misconduct.

- Associate Editor for the Royal Society of Chemistry, RSC Advances (2015-2017), IF ~3 at the time

  Evaluation of 150-200 manuscripts a year from initial editorial assessment, coordination of peer review to final decisions (60-70% overall rejection rate). Worked with RSC staff (located in Cambridge, UK) to address questions from authors and referees.

- Member, Editorial Board of Molecular Simulation, Taylor and Francis (2019-present), IF ~2.5
  Molecular Simulation is a leading journal dedicated to molecular simulation and molecular modelling, including methods developments to solve problems in biology, biochemistry, chemistry, engineering, materials science, medicine, and physics.
- Associate Editor for Taylor and Francis, Clay Minerals (2021 - 2023), and Member of Editorial Board. Occasionally handle a few manuscripts and attend board meetings.
- Guest editor and member of the editorial board of about a dozen other journals (JOM, Surfaces, J. Compos. Sci., J. Theoret. Chem., ISRN Physical Chemistry, Annals of Materials Science and Engineering, Silicon, Acta Chem. Malaysia, Biointerface Research, Austin Biomolecules, IJBMBS)

3) Service for Professional Societies

American Chemical Society (ACS)

- Co-Chair, Communications Committee of the PMSE division (2024-present)
  Owner of the new PMSE web portal, working with an external contractor, PMSE leadership, and a team of committee members to design a new member-only web portal that includes a job board, member forum, awards nomination, symposia proposal submission, award nominations, and access to shared data resources

- Webmaster, PMSE division (2024-present)
  Together with team members, update website content regarding programming, upcoming and past meetings, awards, forms, and special events

- Symposium Organizer (2006-present)
  Organized and co-organized ~10 symposia in PMSE, POLY, COLL, and COMP divisions, several co-sponsored between divisions, and raised symposium support (NSF, DoD, corporate, and CU Boulder)

Materials Research Society (MRS)

- Symposium Organizer (2010-present)
  Organized and co-organized ~5 symposia and raised symposium support (NSF, DoD, corporate, and CU Boulder)

Royal Society of Chemistry (RSC)

- Member, Newton Fellowship Committee (2019-2022)
  Evaluation and selection of candidates for the Newton Postdoctoral Fellowship

The Minerals, Metals & Materials Society (TMS)

- Member, Biomaterials Committee (2018-2022)
  Coordination of 3-4 biomaterials related symposia per year, including an annual symposium on molecular biomimetics (Chair: Candan Tamerler), editing special issues of JOM

Details of Symposia Organized

- MRS Spring Meeting 2025, "Bio/Solid Soft Molecular Interfaces: Biology Meets Materials & Technology" in Seattle, WA, from April 7-11, 2025
  (with Deniz Yucesoy, Izmir Institute of Technology, Yuhei Hayamizu, Tokyo Tech, and Mehmet Sarikaya, U Washington)
- ACS Fall Meeting 2024, Denver, Panel Discussion “Opportunities of AI and Automation in Polymer Research” (Panelists: Pieter in’t Veld, BASF, Gustavo Carri, Exxon, Alan Aspuru-Guzik, U Toronto, Yara Yingling, NCSU, Luke Baldwin, AFRL), August 20th, 2024
- ACS Fall Meeting 2024, Denver, PMSE/COMP Symposium “Navigating the Nanoscale: Innovations in Molecular Dynamics Simulations and Machine Learning for Polymeric Materials” (with Vikas Varshney, AFRL, Ying Li, U Wisconsin-Madison, Andrea Browning, Schrodinger), Denver, CO, August 18-22, 2024
- ACS Spring Meeting 2023, PMSE Symposium “Transcending Nature in the Design of Polymer Hybrid Materials for Structural Applications: Advances in Experiments,

Simulations, and AI Based Design " (with Dhriti Nepal, AFRL, Carole Perry, Nottingham Trent University, UK, Emilie Siochi, NASA Langley Research Center), Indianapolis, IN, March 25-31, 2023

- MRS Spring Meeting 2022, Symposium SF12 "Bioinspired Structural Composites—Advances in Experiments, Simulations and AI-Based Design" (with Dhriti Nepal, AFRL, Carole Perry, Nottingham Trent University, UK, Emilie Siochi, NASA Langley Research Center), Honolulu, HI, May 8-13, 2022
- TMS 2022 National Meeting, Symposium "BioNano Interfaces and Engineering Applications" (with Candan Tamerler, University of Kansas, Kalpana S. Katti, North Dakota State University, Terry C. Lowe, Colorado School of Mines, Po-Yu Chen, National Tsing Hua University), Anaheim, CA, February 27 – March 3, 2022
- Pacifichem 2020/2021, Symposium "Inorganic Oxide and Hydroxide Nanosheets: Toolkits for Structurally and Functionally Designed Nanomaterials" (with Nakato Teruyuki, Kyushu Institute of Technology, Jae-Min Oh, Yonsei University, Miharu Eguchi, NIMS/Japan), Dec 15-20, 2021, Virtual
- TMS 2021 National Meeting, Symposium "Bio-Nano Interfaces and Engineering Applications" (with Candan Tamerler, University of Kansas, Kalpana S. Katti, North Dakota State University, Terry C. Lowe, Colorado School of Mines, Po-Yu Chen, National Tsing Hua University), Virtual, March 15-18, 2021
- MRS Spring Meeting 2020, Symposium CT04 "Tailored Interphases for High Strength and Functional Composites: Advances in Experiments, Simulations, and AI Based Design" (with Dhriti Nepal, AFRL, Luke Henderson, Deakin University, Cheol Park, NASA Langley Research Center), Phoenix, AZ, April 13-17, 2020
- TMS 2020 National Meeting, Symposium "Bio-Nano Interfaces and Engineering Applications" in San Diego, CA, February 23-27, 2020 (with Candan Tamerler, University of Kansas, Kalpana S. Katti, North Dakota State University, Po-Yu Chen, National Tsing Hua University, Terry C. Lowe, Colorado School of Mines)
- ACS Spring National Meeting 2019, PMSE Division, Symposium "Molecular Engineering of Interphases in Polymeric Materials: Advances in Experiments and Simulations" in Orlando, FL, March 31-April 4 (with Dhriti Nepal, Air Force Research Laboratory, Luke Henderson, Deakin University, Reeja Jayan, Carnegie Mellon University)
- TMS 2019 National Meeting, Symposium "Bio-Nano Interfaces and Engineering Applications" in San Antonio, TX, March 10-14 (with Candan Tamerler, University of Kansas, Kalpana S. Katti, North Dakota State University, Po-Yu Chen, National Tsing Hua University, Terry C. Lowe, Colorado School of Mines)
- MRS Fall National Meeting 2015, Symposium WW "Modeling and Theory-Driven Design of Soft Materials" in Boston, MA (with Meenakshi Dutt, Rutgers U, Yara Yingling, North Carolina State U, Tiffany R. Walsh, Deakin U), 4 days
- MRS Spring National Meeting 2015, Symposium GG "Foundations of Bio/Nano Interfaces: Synthesis, Modeling, Design Principles and Applications" in San Francisco, CA (with C. C. Perry, C. Tamerler, Y. Hayamizu), 4 days

- ACS Fall National Meeting 2013, POLY Division, Symposium "Structural Composites and Biomaterials: Modeling and Experiments" in Indianapolis, IN (with J. Moller, R. J. Berry), 20 contributions
- ACS Fall National Meeting 2012, POLY Division, Symposium "Modeling and Simulation of Polymers" in Philadelphia, PA, (with B. L. Farmer, E. Sun, A. Bosse), 50 contributions
- ACS Spring National Meeting 2012, PMSE and COMP Divisions, Symposium "Self-assembled Nanostructures of Biopolymers, Organic Semiconductors, and Inorganics" in San Diego, CA (with R. Berry, J. Luettmer-Strathmann, J. Gilman), 50 contributions
- NSTI Nanotech National Meeting 2011, Symposium "Nano & Micro: Computational Methods, Simulation & Software Tools" (with M. Makowski and S. McGrother), 90 contributions
- ACS Fall National Meeting 2010, PMSE and COMP Divisions, Symposium "Simulation of Hybrid Interfaces and Multi-Component Polymeric Materials", 30 contributions
- ACS Spring National Meeting 2010, POLY Division, Symposium "Synthetic and Biological Macromolecules for Emerging Nanpotechnologies" (with S. Patwardhan), 30 contributions
- ACS Fall National Meeting 2009, PMSE and COMP Divisions, Symposium "Simulation of (Bio)Organic-Inorganic Interfaces and Nanostructures Using MD, MC, and Multiscale Approaches", 30 presenters
- XIV. International Clay Conference 2009, Symposium "Simulation and Theory of Clay Minerals and Interfaces" in Castellaneta Marina, Italy, 30 contributions
- AIChE National Meeting 2008, 3 Sessions "Modeling Composites", "Multifunctional Composites", "Properties and Characterization of Nanocomposites"
- Annual Clay Minerals Society Meeting, 2007, Session "Clay Nanomaterials"

  (with Jeffery Greathouse, Sandia National Laboratories)

4) Reviewer for government agencies and universities

- Panel reviewer for US agencies (2012-present):
  NSF: >27 panels: 2025 (4), 2024 (1), 2023 (1), 2022 (2), 2021 (3), 2020 (2), 2019 (3), 2018 (2), 2017 (3), 2016 (1), 2015 (2), 2014 (1), 2013 (2)
  DoE: 2017 (1)
  NASA: 2016 (1)
  AFRL/UES panel: 2015 (1)

- Reviewer of individual proposals (>150 from 2012) for NSF, AFOSR, NASA, DoE, Army Research Laboratory, ACS-PRF, DFG (Germany), SNSF (Switzerland), Austrian Science Fund, Netherlands Science Organization (NWO), Israel Science Foundation, Kazakhstan Science Foundation

- Reviewer for tenure and promotion cases (2 tenured associate professor, 2 full professor)

5) Reviewer for science and engineering publishers

- Reviewer for scientific journals (>500 times from 2006)
  Including Nature, Nat. Chem., Nat. Mater., Nat. Comm., Adv. Mater, Sci. Adv., Nano Letters, JACS, Angew. Chem. Int. Ed., ACS Nano, ACS Photonics, Chem. Sci., Chem. Comm., Chem. Mater., Soft Matter, J. Phys. Chem. C, J. Chem. Phys., Phys. Chem. Chem. Phys., Chem. Phys. Chem., Macromolecules, Langmuir, Polymer, J. Polym. Sci., J. Coll. Interface Sci., MRS Bulletin, Macromolecular Theory and Simulation, Nat. Comput. Mater., Comput. Mater. Sci., J. Mater. Res., Mechanics of Time Dependent Materials, Polymer International, Polymer Engineering and Science, Microscopy Research and Technique, Chemical Papers, Scientific Reports, ACS Appl. Mater. Interfaces, RSC Advances, New J. Chem.

- Reviewer of book proposals for CRC, Oxford U Press, Nova Science publishers

6) Outreach Activities

- Coordinated and mentored the US National Chemistry Olympiad for the ACS Akron local section from 2009 until 2015

  Organized local exams and national-level exams for High School students in a three-county area with 72 High Schools every year. Participation was about 50 students in the first round for a half day event and 10 students in the second round for a full day event, which included on-site laboratory practicals and help by several TAs.

- Organized a Biannual Engineering Career Day at the University of Akron 2008-2015
  The events were held for High School students, teachers, and parents and involved presentations by professionals and undergraduates, Q&A sessions, and an informal reception (50-70 participants)

- Engaged graduate students to visit Elementary Schools and Middle Schools in Boulder/Denver for presentations to children and teachers during 2016-present