

## Hendrik Heinz

Professor

Department of Chemical and Biological Engineering

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## 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
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## Honors and Awards

- 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 (14<sup>th</sup> 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
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**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 (Langmuir) 04/2021 – present
  - Amazon Scholar, Amazon 08/2022 – 2023
  - Consultant, Amazon 10/2021 – 07/2022
  - Associate Editor, Royal Society of Chemistry/CNRS (New Journal of Chemistry) 10/2017 – 03/2021
  - Associate Editor, Royal Society of Chemistry (RSC Advances) 10/2015 – 10/2017
  - 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
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**Publications in Peer-Reviewed Journals and Book Chapters**

H index 53, >11300 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

**Papers in Preparation (selected) and Under Review**

140. "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. (under re-review)
139. “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. (under re-review)
138. “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. (under re-review)
137. “Force Field Parameters for Lithium Cobalt Oxide and Multiphase Battery Materials”  
Liu, J. (PD); Cui, Q.; **Heinz, H.** (\*) &
136. “Understanding the Effect of Peptide 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.** (\*) &
135. „Prediction of Carbon Nanostructure Mechanical Properties Using Reactive Simulations and  
Machine Learning“  
Winetrou, J. J. (GS); Zhao, Q.; Wang, Y. (\*); **Heinz, H.** (\*) &  
Adv. Mater. (Under re-review)
134. „Reactive Molecular Dynamics Simulations with the Interface Force Field (IFF-R)“  
Winetrou, J. J. (GS); Kanhaiya, K. (GS); Sachdeva, G.; Odegard, G. M.; **Heinz, H.** (\*) &  
Nat. Comm. (Under re-review)
133. “Understanding Phase Equilibria, Mechanical, Thermal, and Organic Interfacial Interactions  
of Calcium Sulfate Minerals at the Atomic Scale”  
Mishra, R. K. (GS); Flatt, R. J.; **Heinz, H.** (\*) &  
Cem. Concr. Res. (Under re-review)

### **Published/Accepted**

- 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](https://doi.org/10.1021/acs.langmuir.3c02948) (IF 4)
131. “Analyzing the Li–Al–O Interphase of Atomic Layer-Deposited Al<sub>2</sub>O<sub>3</sub> 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](https://doi.org/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](https://doi.org/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](https://doi.org/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); **Heinz, H.** (\*) &  
ACS Nano 2023, 17, 9938-9952. DOI: [10.1021/acsnano.2c10953](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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.2106965119](https://doi.org/10.1073/pnas.2106965119) (IF 11)
121. „Binding of Polar and Hydrophobic Molecules at the LiCoO<sub>2</sub> (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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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.; Winetroun, 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); Winetroun, J. J. (GS); **Heinz, H.**; Shah, S.; Maiaru, M. &  
Macromolecules 2021, 54, 9815-9824. [DOI: 10.1021/acs.macromol.1c01813](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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); Winetrou, J. (GS); Flatt, R. J.; **Heinz, H. (\*)** &  
Cem. Concr. Res. 2021, 139, 106262. [DOI: 10.1016/j.cemconres.2020.106262](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1126/sciadv.aaz7188) (IF 12)
96. “Reactive Modeling of Mo<sub>3</sub>Si 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](https://doi.org/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](https://doi.org/10.1039/C9GC03287H) (IF 9.4)  
(Cover Art, Mar 7:  
<https://pubs.rsc.org/en/content/articlelanding/2020/gc/d0gc90026c/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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”  
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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”  
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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.  
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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. (\*)  
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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. (\*)  
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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](https://doi.org/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.** (\*) &  
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Zartman, G. D. (UGS); Liu, H. (GS); Akdim, B.; Pachter, R.; **Heinz, H.** (\*) &  
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22. "Computational Screening of Biomolecular Adsorption and Self-Assembly on Nanoscale Surfaces"  
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- 21.\* "Synthesis, Structure, Characterization, and Properties of Organically Modified Layered Silicates"  
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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.  
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- 19.\* "Molecular Models and Simulations of Layered Materials"  
Cygan, R. T. (\*); Greathouse, J. A.; **Heinz, H.**; Kalinichev, A. G.  
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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](https://doi.org/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. (\*)  
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**Heinz, H.** (\*); Vaia, R. A.; Farmer, B. L.; Naik, R. R.  
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**Heinz, H.** (\*); Vaia, R. A.; Koerner, H.; Farmer, B. L.  
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  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.  
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  - 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](https://doi.org/10.1080/08927020701308828) (IF 1.7)
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**Heinz, H.** (\*); Vaia, R. A.; Krishnamoorti, R.; Farmer, B. L.  
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  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. (\*)  
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**Heinz, H.** (\*); Vaia, R. A.; Farmer, B. L.  
J. Chem. Phys. 2006, 124, 224713. [DOI: 10.1063/1.2202330](https://doi.org/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](https://doi.org/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.  
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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](https://doi.org/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](https://doi.org/10.1063/1.1642605) (IF 3.0)
  5. "Surface Structure of Organoclays"  
**Heinz, H.**; Suter, U. W. (\*)  
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  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](https://doi.org/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](https://doi.org/10.1021/ja021248m) (IF 15)
  2. "Simple and Accurate Computations of Solvatochromic Shifts in  $\pi \rightarrow \pi^*$  Transitions of Aromatic Chromophores"  
**Heinz, H.**; Suter, U. W.; Leontidis, E. (\*)  
J. Am. Chem. Soc. 2001, 123, 11229-11236. [DOI: 10.1021/ja010396u](https://doi.org/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](https://doi.org/10.1063/1.1342238) (IF 3.0)
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## 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.
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## 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 Nanoparticles – 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.

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### 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 MoS<sub>2</sub>), 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”

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### **Undisclosed Proprietary Work**

1. Heinz, H. (for Sika AG, Zürich), 2004  
“Modeling of organic oligomers on mineral surfaces”

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### **Invited Talks & Seminars (\* Plenary)**

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 25<sup>th</sup>, 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” · 10<sup>th</sup> 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” · Pacificchem 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“ · 4<sup>th</sup> 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, Dübendorf, 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 Photoreponses of Switchable Azobenzene Derivatives and Alkylammonium Surfactants in Clay Interlayer Spaces“ · 16<sup>th</sup> 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 13<sup>th</sup> Freiburger Symposium · 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“ · 5<sup>th</sup> 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 Sn<sup>2+</sup>/Zn<sup>2+</sup> 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” · 6<sup>th</sup> 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, Department 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" · 2<sup>nd</sup> 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” · 7<sup>th</sup> 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” · 2<sup>nd</sup> International Symposium on Stimuli-Responsive Materials · University of Southern Mississippi · Hattiesburg, MS · Oct 31, 2007
24. “Peptide Binding to Sheet Silicate and Metal Nanoparticles – 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" · 44<sup>th</sup> 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 Models" Academia 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 168<sup>th</sup> 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

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

- 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 Winetroun 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<sub>2</sub>O<sub>3</sub> 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<sup>th</sup> 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 Winetrou 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 sp<sup>3</sup> 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 Winetrou 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 Winetrou 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 Winetrou and Sagar Patil)
- 185.T „Accurate Molecular Models for MoS<sub>2</sub> 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 MoS<sub>2</sub> 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 Polylysine Acetate 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. Gissing)
- 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“ · 16<sup>th</sup> 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’Espinoise de Lacaille)
- 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<sub>3</sub>Si (A15) Oxidation and Resulting Silica Morphology” · MURI Review, University of Virginia · Charlottesville, VA · Jun 29, 2016 (by Chamila Dharmawardhana)
- 133.P “MoSi<sub>2</sub> 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 Gissing)
- 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 Single 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-Polymer 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” · 13<sup>th</sup> 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” · 13<sup>th</sup> 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” · 14<sup>th</sup> 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” · 14<sup>th</sup> 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 Nanoparticle 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-Planck-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 · 93<sup>rd</sup> 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 Cementitious 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—7<sup>th</sup> 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” · 20<sup>th</sup> 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 Francini 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	3	Chemical Engineering Materials	100	CHEN 4440	Spring 2017-2024
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 1<sup>st</sup> and 2<sup>nd</sup> 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).

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## Mentoring

- **Advisor of postdocs:**

10. Dr. Cheng Zhu, 09/2019 – 08/2023
9. Dr. Juan Liu, 07/2016 – 07/2019, subsequently full 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, Michigan Tech U
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, Virginia Tech
2. Dr. Jie Feng, 2008-2011, NETL Pittsburgh
1. Dr. Pratyush Dayal, 2007-2008, IIT Gandhinagar

- **Advisor of PhD students:**

Current:

16. Leo Beck, 10/2023-present  
Hybrid organic-inorganic structures for photovoltaics and LEDs
15. Isaac Armstrong, 09/2020-present  
CO<sub>2</sub> capture in ionic liquids and polymer structures
14. Jordan Winetrout, 08/2019 – present, graduation expected Spring 2024  
Designing ultrastrong carbon-based composites using simulations and data science

Graduated:

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, Passed 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”
- **PhD Students advised at U Akron who remained at U Akron upon relocation to CU Boulder, changing advisors and completing 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:**
    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<sub>x</sub> 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), 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. Peiyong 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):**

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
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, U.S. patent office, postdocs (Institute Pasteur/CNRS (France), U Chicago, Georgia Tech, Northwestern U), faculty (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, IIT Gandhinagar, Dalian Maritime University), government (NETL), industry (Tata Steel, Sherwin Williams), 2nd postdocs (George Washington U, Michigan Tech U)
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## 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
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## Service

### 1) Service to the Department, College, and University

University of Colorado Boulder (2015-present):

- Chair of investigation committee for research misconduct (2023-2024)  
Leading the investigation into research misconduct by a group of PIs at CU Boulder in collaboration with the VP for research compliance and two committee members
- Executive committee for Annual Boulder Frontiers Symposium (2019-2022)  
Leadership in planning for the annual ChBE symposium
- Department Faculty Committee (2018-2020)  
Faculty recruiting (including diversity), faculty awards, mentoring, reappointment, promotion and tenure reviews, and recommendations for improving the faculty experience.
- Department Faculty Search Committee (2015-2018)  
Reviewed candidate files, preparing rankings and recommendations to select candidates for interviews. Hosted faculty candidates and discussed feedback.

- Support in graduate student recruiting (2016-2018)  
Led several groups of incoming PhD recruits to meals and supported the admissions committee.
- Member of Dissertation/Thesis Committees  
Serving/served on several PhD thesis committees, including James Wertz (ChBE), Pengxiao Hao (ChBE), Mengyuan Wang (MSE), Gopal Ramalingam (University of Virginia, Advisor: Prof. Petra Reinke).
- Member of 10+ Ph.D. Qualifying Exam Committees

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

i) Within the Department of Polymer Engineering

- Department Visitation Committee, Chair (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.
- Department Admissions Committee, Member (2007-2014)  
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.
- Department Curriculum Committee, Member (2008-2014)  
Evaluated and contributed to changes in curriculum.
- Bayer Lectureship Committee, Member (2009-2012)  
Identifying speakers, coordination of visit
- Served on 3 PhD thesis committees as non-principal advisor during 2012-2015.
- 25<sup>th</sup> Anniversary Organization Committee of DPE (2007-2008)

iii) Within the University

- University Curriculum Committee (2008-2010)
- Curriculum Committee of the Graduate Council (2007-2008)
- Provost Advisory Committee (2008-2010)
- 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 Langmuir – the ACS journal of colloids and interfaces (2021- present)  
Handling ~200 manuscripts a year from initial assessment, selection of referees and coordination of peer review through revisions and decisions (~60% overall rejection rate). Participation in editorial conferences and working with ACS staff to address questions from

authors and referees. Further development of the journal and advising in cases of ethical misconduct.

Langmuir is the leading journal of interfacial and colloidal chemistry published by the American Chemical Society. It publishes high-quality, original, and significant work in the science and application of systems and materials in which the interface dominates structure and function (IF 3.8).

- Member of editorial board of Molecular Simulation (2019-present). Molecular Simulation is a leading journal dedicated to molecular simulation, molecular modelling, and often associated methods developments that help solve problems in biology, biochemistry, chemistry, engineering, materials science, medicine, and physics (IF 2.2).
- Associate editor for Clay Minerals (2021 - present) and Member of Editorial Board. Occasionally handle a few manuscripts and attend board meetings.

Earlier Guest Editor for Clay Minerals (2017/2018): Handled several manuscripts for a special issue as a service to the Mineralogical Society.

- Associate editor for New J. Chem. (2017-2021)

Handled 300-400 manuscripts a year from initial assessment, selection of referees and coordination of peer review through revisions and decisions (60-70% overall rejection rate). Participation in editorial conferences and 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.

New Journal of Chemistry is a broad primary journal for all branches of chemistry, owned by CNRS, and published by the Royal Society of Chemistry, UK. It publishes high-quality, original and significant work with an emphasis on contributions that open new directions in chemistry (IF 3.6).

- Associate editor for RSC Advances (2015-2017)

Handled 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.

RSC Advances is an international, peer-reviewed journal covering all of the chemical sciences, including multidisciplinary and emerging areas. Work must be high quality and advance the field (IF 3.1).

- Editor of Book “Self-Assembled Nanostructures of Biopolymers, Organic Semiconductors, and Inorganics” (Wiley & Sons). 10-15 chapters by leading researchers in the field.
- Member of the editorial board of several journals (New J. Chem., Molecular Simulation, 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

- TMS: Member of the Biomaterials Committee (2018-present)  
Helping in coordination of 3-4 biomaterials related symposia per year, specifically the organization of an annual symposium on molecular biomimetics (Chair: Candan Tamerler), and editing special issues of JOM.

- Royal Society of Chemistry: Member of the Newton Fellowship Committee (2019-present)  
I help evaluate and select candidates for the Newton Postdoctoral Fellowship

#### 4) Reviewer for government agencies and universities

- Panel reviewer for US agencies (2012-present):  
NSF panels served: 16 – 2 (2020), 3 (2019), 2 (2018), 3 (2017), 1 (2016), 2 (2015), 1 (2014), 2 (2013)  
DoE panels served: 1 (2017)  
NASA panels served: 1 (2016)  
Air Force Research Laboratory/UES panel: 1 (2015)
- 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) Symposia Organized and in Progress

I co-organized 8 multi-day symposia at professional society meetings since 2017

In progress:

- MRS Fall Meeting 2024, Boston, TBA
- 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

Completed:

- 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
- Pacificchem 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, Miharuru 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, Reejay 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. Luettmmer-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 Nanotechnologies” (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”

#### **6) Reviewer for science and engineering publishers**

- Reviewer for scientific journals (>400 times from 2012)  
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

#### **7) 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
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