
Hendrik Heinz

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Education

- Air Force Research Laboratory, WPAFB, OH 08/2006
Postdoctoral
Modeling of (bio)nanostructured materials
 - ETH Zurich, Switzerland 06/2003
Ph.D. in Materials Science and Engineering
Simple energy models and simulation of organically modified silicates
Advisors: Prof. Ulrich W. Suter · Prof. Hans-Christian Oettinger
 - M.Sc. (Diploma) in Chemistry 09/2000
Calculation of solvatochromic shifts of perylene in n-alkane matrices
Advisors: Prof. Ulrich W. Suter · Prof. Epameinondas Leontidis (University of Cyprus)
 - University of Heidelberg, Germany 09/1997
B.Sc. (Prediploma) in Chemistry
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Honors

- Giovanni Novelli Prize (14th Int. Clay Conf., Italian Clay Group) 2009
 - HP Outstanding Junior Faculty Award (ACS, COMP Division) 2006
 - Member of the “AFOSR Star Team” (PI R. A. Vaia) 2005
 - Graduate Scholarship of the German National Academic Foundation 2001–2003
 - Undergraduate Scholarship of the German National Academic Foundation 1995–2000
 - Silver medal at the 26. International Chemistry Olympiad, Oslo, Norway 1994
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Appointments

- Assistant Professor 09/2006 – present
University of Akron · Ohio · Department of Polymer Engineering
Computer simulation · Inorganic-organic interfaces · Biomineralization
Charge transport · Self-assembly on metal surfaces

- Consultant 04/2004 – present
Sika Corporation · Switzerland
Computer simulation · Models for inorganic solids, polymers, and polyelectrolytes
 - Post-Doc 02/2004 – 08/2006
Air Force Research Laboratory · Dayton · Ohio (B. L. Farmer, R. A. Vaia)
Computer simulation of nanostructured materials at atomistic and coarse-grained level
Polymer-layered silicate nanocomposites · Bioinspired Materials · Actuators
 - Research Associate 09/2003 – 01/2004
ETH Zurich · Sika Corporation · Zurich · Switzerland (N. Blank, R. Flatt)
Pilot project to develop computational models and methods to study interfaces between (semi)metal oxide surfaces, charged organic polymers, and PEO
 - Visiting Scientist 05/2001 – 12/2003
University of Mainz · Germany (K. Binder, W. Paul) (part-time)
Computational analysis of phase transitions in polymer brushes · Development of a method to calculate local pressures in systems with many-body interactions
 - Research Assistant 02/2001 – 08/2003
ETH Zurich · Switzerland (U. W. Suter, H. C. Oettinger)
Improved concept to assign atomic charges for classical simulations of polar systems
Explanation of phase transitions and self-assembly patterns of alkyl chains on mica based on simulation and experimental data/measurements · Extension of force fields for organic molecules (PCFF) to simulate inorganic-organic interfaces with mica
 - Graduate Researcher 05/2000 – 08/2000
University of Cyprus · Nicosia · Cyprus (E. Leontidis)
Experimental and theoretical investigation of π - π^ solvatochromic spectral shifts of perylene in n-alkane matrices*
 - Project Assistant 04/1993 – 06/1994
Technical University of Chemnitz · Chemnitz · Germany (G. Marx) (part-time)
Analysis of metallic alloys using Glow Discharge Optical Emission Spectrometry
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Publications in Peer-Reviewed Journals (* invited)

27. “Atomistic Simulation of Poly(ethylene oxide) in Aqueous Solution: Challenges and Suggestions for Models”
Heinz, H.; Schober, I.; Flatt, R. J. (in preparation)
26. “Adsorption of Amino Acids and Surfactants on Au {111} Surfaces in Aqueous Solution”
Feng, J.; Naik, R. R.; Farmer, B. L.; Heinz, H. (in preparation)
25. “Polarization at Metal-Biomolecular Interfaces”
Jha, K. C.; Naik, R. R.; Farmer, B. L.; Heinz, H. (in preparation)
24. “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.; Heinz, H. (submitted)
- 23.* “Structure and Cleavage Energy of Surfactant-Modified Clay Minerals: Influence of CEC,

- Head Group, and Chain Length”
Fu, Y. T.; Heinz, H.
Phil. Mag. 2010 (submitted)
22. “Nanoscale Tensile, Shear, and Failure Properties of Layered Silicates as a Function of Cation Density and Stress”
Zartman, G. D.; Heinz, H. (submitted)
 21. “Computational Screening of Biomolecular Adsorption and Self-Assembly on Nanoscale Surfaces”
Heinz, H.
J. Comp. Chem. 2009 (accepted).
 20. “Nature of Molecular Interactions of Peptides with Gold, Palladium, and Pd-Au Bimetal Surfaces in Aqueous Solution”
Heinz, H.; Farmer, B. L.; Pandey, R. B.; Slocik, J. M.; Patnaik, S. S.; Pachter, R.; Naik, R. R.
J. Am. Chem. Soc. 2009, 131, 9704–9714. [PDF](#)
 19. “Molecular Models and Simulations of Layered Materials”
Cygan, R. T.; Greathouse, J. A.; Heinz, H.; Kalinichev, A. G.
J. Mater. Chem. 2009, 19, 2470–2481. Journal Cover. [PDF](#)
 - 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.; Farmer, B. L.; Slocik, J. M.; Drummy, L. R.; Naik, R. R.
Phys. Chem. Chem. Phys. 2009, 11, 1989–2001. Inv. Paper. [PDF](#)
 17. ”Towards Understanding Amino Acid Adsorption at Metallic Interfaces: A Density Functional Theory Study”
Hong, G.; Heinz, H.; Naik, R. R.; Farmer, B. L.; Pachter, R.
ACS Appl. Mat. Interf. 2009, 1, 388–392. [PDF](#)
 16. “Accurate Simulation of Surfaces and Interfaces of FCC Metals Using 12-6 and 9-6 Lennard-Jones Potentials”
Heinz, H.; Vaia, R. A.; Farmer, B. L.; Naik, R. R.
J. Phys. Chem. C 2008, 112, 17281–17290. [PDF](#)
 15. „Photoisomerization of Azobenzene Grafted to Montmorillonite: Simulation and Experimental Challenges”
Heinz, H.; Vaia, R. A.; Koerner, H.; Farmer, B. L.
Chem. Mater. 2008, 20, 6444–6456. [PDF](#)
 14. “Relation between Packing Density and Thermal Transitions of Alkyl Chains on Layered Silicate and Metal Surfaces”
Heinz, H.; Vaia, R. A.; Farmer, B. L.
Langmuir 2008, 24, 3727–3733. [PDF](#)
 - 13.* “Calculation of Local and Average Pressure Tensors in Molecular Simulation”
Heinz, H.
Molecular Simulation 2007, 33, 747–758. [PDF](#)
(Special issue: Recent Developments in Molecular Simulation)
 12. “Self-Assembly of Alkylammonium Chains on Montmorillonite: Effect of Chain Length, Headgroup Structure, and Cation Exchange Capacity”
Heinz, H.; Vaia, R. A.; Krishnamoorti, R.; Farmer, B. L.
Chem. Mater. 2007, 19, 59–68. [PDF](#)
 11. ”Dynamics of Alkyl Ammonium Intercalants within Organically Modified Montmorillonite: Dielectric Relaxation and Ionic Conductivity”

- Jacobs, J. D.; Koerner, H.; Heinz, H.; Farmer, B. L.; Mirau, P. A.; Garrett, P. H.; Vaia, R. A.
 J. Phys. Chem. B 2006, 110, 20143–20157. [PDF](#)
10. "Interaction Energy and Surface Reconstruction between Sheets of Layered Silicates"
 Heinz, H.; Vaia, R. A.; Farmer, B. L.
 J. Chem. Phys., 2006, 124, 224713. [PDF](#)
 9. "Calculation of Local Pressure Tensors in Systems with Many-Body Interactions"
 Heinz, H.; Paul, W.; Binder, K.
 Phys. Rev. E, 2005, 72, 066704. [PDF](#)
 8. „Force Field for Phyllosilicates and Dynamics of Octadecylammonium Chains Grafted to Montmorillonite“
 Heinz, H.; Koerner, H.; Vaia, R. A.; Anderson, K. L.; Farmer, B. L.
 Chem. Mater. 2005, 17, 5658–5669. [PDF](#)
 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. [PDF](#)
 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. [PDF](#)
 5. "Surface Structure of Organoclays"
 Heinz, H.; Suter, U. W.
 Angew. Chem. Int. Ed. 2004, 43, 2239–2243. [PDF](#)
 4. "Atomic Charges for Classical Simulations of Polar Systems"
 Heinz, H.; Suter, U. W.
 J. Phys. Chem. B 2004, 108, 18341–18352. [PDF](#)
 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. [PDF](#)
 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. [PDF](#)
 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. [PDF](#)
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Contributions to Books

6. "Alkylammonium Chains on Layered Silicate Surfaces"
 Heinz, H. In "Rubber-Clay Nanocomposites: Science, Technology and Applications"; Galimberti, M., ed.; Wiley and Sons 2010 (in progress).
5. "Modification of inorganic fillers and interfacial properties in polyolefin nanocomposites: Theory versus Experiment"

- Feng, J.; Heinz, H. In "Advances in Polyolefin Nanocomposites"; Mittal, V., ed.; CRC Press 2010 (in progress).
4. "Molecular Simulation and Thermodynamics of Polymer Blends and Melts"
Virnau, P.; Binder, K.; Heinz, H.; Kreer, T.; Müller, M., In "Encyclopedia of Polymer Blends", Isayev, A. I., ed., Volume 1 "Fundamentals", Wiley-VCH 2009 (in press).
 3. "Understanding Clay Surface Modification and Organic-Inorganic Interfaces"
Heinz, H. In "Advances of Polymer Nanocomposite Technology", Mittal, V., ed., Nova Science 2009 (in press).
 2. "Simulation of Nanocomposites"
Patnaik, S. S; Heinz, H.; Pandey, R. B.; Farmer, B. L. In "Modeling and Simulation of Polymers"; Leonov, A. I., Gujrati, P. D, eds.; Wiley-VCH 2009 (in press).
 1. "Synthesis, Structure, Characterization, and Properties of Organically Modified Layered Silicates"
Heinz, H. In "Nanocomposites"; Beyer, G., ed.; AMI: Bristol, 2009. ISBN 9781906479046.
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Patents

2. Heinz, H. "Methods and Systems for the Accurate Atomistic Simulation of Poly(ethylene oxide) in Aqueous Solution" Preliminary Patent Application (2009).
 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

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”
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.

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)

43. “Nanoscale Linear Mechanical and Cleavage Properties of Layered Silicates” · Sandia National Laboratories · Albuquerque, NM · Sep 22, 2009
42. “Interaction of Protein Building Blocks and Surfactants with Shaped Surfaces of Au, Pd, and Silica in Aqueous Solution” · AFRL/RX Biotech Review, WBI · Dayton, OH · Sep 15, 2009
41. “Interaction of Protein Building Blocks and Surfactants with Shaped Surfaces of Au and Pd Nanostructures in Solution” · University of Akron, Department of Polymer Science · Akron, OH · Sep 3, 2009
40. “Functional Interfaces of Silicates with Peptides and Polymers Guided By Molecular Simulation” · ACS Fall National Meeting · Washington, DC · August 19, 2009
39. “Interaction of Protein Building Blocks and Surfactants with Shaped Surfaces of Au and Pd Nanostructures in Solution” · University of Patras (Greece) · Department of Chemical Engineering · June 29, 2009
38. “Interaction of amino acids, surfactants, and peptides with even, stepped, and spherical surfaces of gold and palladium nanostructures in aqueous solution” · AFRL/RX Research Meeting · Wright-Patterson AFB, OH · May 29, 2009
37. “Simulation of FCC Metals and Metal-Biological Interfaces for Nanoelectronic and Sensor Applications” · NIST · Workshop on Atomistic Simulations for Industrial Needs · Gaithersburg, MD · Apr 27, 2009
36. “Design of Functional Nanoparticle Interfaces and Polyelectrolytes Guided By Atomistic Simulation” · Int. Conf. on High Tech Mat. 2009 · IIT Kharagpur, India · Feb 12, 2009
35. “Molecular Dynamics Simulation of Poly(ethylene oxide) and Clay Mineral Interfaces with Surfactants and Peptides In Aqueous Solution” · Procter & Gamble · Cincinnati, OH · Dec 19, 2008
34. “Modeling the Interaction of Peptides and Surfactants with Inorganic Surfaces: Understanding Specificity Through Computation and Experiment” · Dept Seminar Chemistry · Nottingham Trent Univ · Nottingham, UK · Nov 5, 2008
33. “Adsorption of Single Amino Acids and Surfactants to Au {111} Surfaces in Aqueous Solution - Insight from Atomistic Simulation” · Dept Seminar Physics · Univ of South Mississippi, MS · Oct 31, 2008

- 32.* “Design of Functional Nanoparticle Interfaces and Polyelectrolytes Guided By Atomistic Simulation” · Int. Conf. on Stimuli-Responsive Materials · Hattiesburg, MS · Oct 29, 2008
31. “Nanomechanics and Energetics of Layered Silicates for Nanocomposites” · ACS Rubber Tech Meeting and Expo · Louisville, KY · Oct 15, 2008 (given by J. Feng)
30. “Simulation of Metals and Metal-Biological Interfaces for Sensor and Nanoelectronic Applications” · Dept Seminar Math and Applied Math · Univ of Akron, OH · Oct 2, 2008
29. “Atomistic Simulation of PEO in Solution – Challenges and New Models” · University of Mainz, Germany · Condensed Matter Physics Seminar · June 24, 2008
28. “Peptide Binding to Inorganic Surfaces and Thermal Transitions of Alkyl Chains on Nanoparticle Surfaces: Computation and Experiment” · ACS Central Regional Meeting · Columbus, OH · June 11, 2008
27. “Simulation of Inorganic-(bio)organic Interfaces and Thermal Transitions of Alkyl Chains on Surfaces” · Smart Coatings 2008 · Orlando, FL · Feb 27, 2008
26. “Molecular Simulation of Inorganic-Biological Interfaces and Optically Switchable Materials” · 7th Int. Conf. on Adv. Polymers for Macromol. Eng. (APME) · Miami, FL · Dec 17, 2007
- 25.* “Atomistic Simulation of Inorganic-Biological Interfaces and Optically Switchable Materials” · 2nd International Symposium on Stimuli-Responsive Materials · University of Southern Mississippi · Hattiesburg, MS · Oct 31, 2007
24. “Peptide Binding to Sheet Silicate and Metal Nanonoparticles – Insight from Atomistic Simulation” · SAMPE Fall Technical Meeting · Cincinnati, OH · Oct 30, 2007
23. “Effective Atomistic Models for Inorganic-Biological Interfaces and Optically Switchable Materials” · Kent State University, Dept of Chemistry · Kent, OH · Sep 06, 2007
22. “Influence of Peptide Sequence on Adsorption on Au, Pd, and Montmorillonite Nanoparticle Surfaces - Insight from Atomistic Simulation” · WPAFB, AFRL/ML, Dayton, OH · Aug 14, 2007
21. “A force field for layered silicates and simulation of interfaces with surfactants and peptides” · 44th Annual Meeting of the Clay Minerals Society · Santa Fe · NM · June 6, 2007
20. “Simulation of Hybrid Materials and Interfaces: Insight from Atomistic and Coarse-grain Models” · ORNL · Chemical Sciences Division · Knoxville, TN · Mar 6, 2007
19. “Peptide Design for Binding to Metal Surfaces Using Atomistic Simulation” · WPAFB, AFRL/ML, Dayton, OH · Feb 20, 2007
18. “Force Fields for Sheet Silicates and Metals” · Accelrys User Meeting and Conference Baltimore, MD · Nov 15, 2006
17. “Simulation of Nanostructured Materials Using Atomistic and Coarse Grain Models” University of Central Florida · Nanoscience and Technology Center · Orlando, FL · Apr 26, 2006
16. “Simulation of Nanostructured Materials Using Atomistic and Coarse Grain Models” University of Akron · Dept. of Polymer Engineering · Akron, OH · Apr 18, 2006
15. “Simulation of Nanostructured Materials Using Atomistic and Coarse-Grain Models” Florida State University · Dept. of Chemical and Biomedical Engineering · Tallahassee, FL · Mar 14, 2006
14. “Simulation of Organic-Inorganic Interfaces Containing Sheet Silicates” · Los Alamos National Laboratory · Theory Division · Los Alamos, NM · Feb 15, 2006
13. “Simulation of Organic-Inorganic Interfaces Using Atomistic and Coarse Grain 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 168th Technical Meeting · Pittsburgh, PA · Nov 1, 2005
8. "Self-assembly of alkylammonium chains on montmorillonite: Effect of chain length, head group structure, and cation exchange capacity" · AFRL/ML, WPAFB · Polymer Branch Research Seminar · Oct 7, 2005
7. "Molecular Modeling of Superplasticizers in Cementitious Systems: Progress" · Sika Technology AG · Zurich, Switzerland · Apr 12, 2005
6. "Energy Models and Atomistic Simulation of Clays with Surface-Grafted Alkylammonium Chains" · MIT · Atomistic Modeling and Simulation Seminar (AMASS) Cambridge, MA · Nov 29, 2004
5. "Modeling Single Molecule Spectral Shifts and Organically Modified Silicates" · ETH Zurich, Swiss Center for Scientific Computing · Computational Chemistry Seminar (M. Parrinello) · Manno, Switzerland · Sep 24, 2003
4. "Simple Energy Models and Simulation of Organically Modified Silicates" · University of Akron · Department of Polymer Science · Polymer Science Colloquium · Aug 19, 2003
3. "Simple Energy Models and Simulation of Organically Modified Silicates" · Air Force Research Laboratory, Wright-Patterson AFB · Materials Science and Technology Colloquium · Dayton, OH · Aug 15, 2003
2. "Partial Charges in Polar Solids" · University of Mainz · Department of Physics · Seminar on Condensed Matter Theory · Mainz, Germany · Dec 3, 2002
1. "Molecular Modeling of Dye-doped Hydrocarbons" · ETH Zurich · Institute of Quantum Electronics · Group Seminar Prof. H. Baltes · Zurich · Jan 20, 2001

Conference Contributions (Talks, Posters incl. coworkers)

- 66.T "Directed Self-assembly of Block Copolymers on Topological Substrates: A Monte Carlo Simulation" · ACS Fall National Meeting · Washington, DC · Aug 19, 2009 (given by J. Feng)
- 65.T "Quantifying Adsorption of Amino Acids and Surfactants on Au {111} Surfaces in Aqueous Solution" · ACS Fall National Meeting · Washington, DC · Aug 19, 2009 (given by J. Feng)
- 64.T "Nature of Molecular Interactions of Peptides With Gold, Palladium, and Pd-Au Bimetal Surfaces in Aqueous Solution" · ACS Fall National Meeting · Washington, DC · Aug 17, 2009
- 63.T "Accurate Simulation of Layered Silicates and Their Interfaces" · 14th Int. Clay Conf. · Castellaneta Marina, Italy · Jun 18, 2009
- 62.T "Structure and Cleavage Energy of Surfactant-Modified Clays: Influence of CEC, Head Group, and Chain Length" · 14th Int. Clay Conf. · Castellaneta Marina, Italy · Jun 14, 2009

- 61.P “Trends in Cleavage Energies of Alkylammonium-Modified Layered Silicates as a Function of Cation Density, Head Group Structure, and Chain Length” · Y. T. Fu, HH et al. · APS March Meeting · Pittsburgh, PA · Mar 16–20, 2009
- 60.P “Quantifying Polarization at Metal-Biological Interfaces in Solution” · K. C. Jha, HH et al. · APS March Meeting · Pittsburgh, PA · Mar 16–20, 2009
- 59.P “Simulation of Peptide Binding to Silica and Silica Mineralization” · F. S. Emami, HH et al. · APS March Meeting · Pittsburgh, PA · Mar 16–20, 2009
- 58.T “Atomistic Simulation of Cleavage Energy of C3S and Organic-silicate Interactions” · R. K. Mishra, HH et al. · NanoCem Workshop · Derio, Spain · Mar 3, 2009
- 57.T “Peptide Binding to Metal, Bimetal, and Layered Silicate Even Surfaces” · MRS Fall Meeting · Boston, MA · Dec 1, 2008 (given by R. B. Pandey)
- 56.T “Adsorption of Single Amino Acids and Surfactants to Au {111} Surfaces In Aqueous Solution - Insight from Atomistic Simulation” · AIChE Annual Meeting · Philadelphia, PA · Nov 20, 2008 (given by J. Feng)
- 55.T “Atomistic Simulation of Poly(ethylene oxide) In Aqueous Solution: Challenges and Suggestions for Models” · AIChE Annual Meeting · Philadelphia, PA · Nov 17, 2008 (given by J. Feng)
- 54.P “Design of Functional Nanoparticle-Peptide Interfaces Guided By Atomistic Simulation” · AFOSR Biotech Review · Arlington, VA · Nov 12/13, 2008 (given by R. J. Berry)
- 53.P G. D. Zartman & HH: “Calculation of Nanoscale Elastic, Shear, and Bending Properties of Sheet Silicates Using Molecular Dynamics Simulation” · PINO Meeting · Case Western Reserve University, OH · Jul 3, 2008
- 52.T “A Force Field for Layered Silicates and Simulation of Interfaces with Surfactants: Structure, Surface Energy, and Phase Transitions” · PPS-24 · Salerno, Italy · June 18, 2008
- 51.T “Peptide Binding to Sheet Silicate and Metal Nanoparticles: Insight from Atomistic Simulation and Experiment” · PPS-24 · Salerno, Italy · June 17, 2008
- 50.T Y. T. Fu & HH: “Modification of surface energies of layered silicates through surfactants of different chain length” · ACS National Meeting · New Orleans, LA · Apr 9, 2008
- 49.T “Peptide Binding to Sheet Silicate and Metal Nanoparticles - Insight from Atomistic Simulation” · ACS Spring Meeting · New Orleans, LA · Apr 06, 2008 (B. L. Farmer)
- 48.T “Photoisomerization of Azobenzene: A Quantitative Force Field-based Implementation and Simulation of Assemblies with Layered Silicates in Comparison with Experiment” · ACS Spring Meeting · New Orleans, LA · Apr 06, 2008
- 47.T “Relation between Packing Density and Thermal Transitions of Alkyl Chains on Layered Silicate and Metal Surfaces” · MRS Spring Meeting · San Francisco, CA · Mar 27, 2008
- 46.P G. D. Zartman & HH: “Calculation of Nanoscale Elastic, Shear, and Bending Properties of Sheet Silicates Using Molecular Dynamics Simulation” · MRS Spring Meeting · San Francisco, CA · Mar 27, 2008
- 45.P K. C. Jha & HH: “Polarization Effect at Peptide-Gold Interfaces Estimated by MD Simulation” · MRS Spring Meeting · San Francisco, CA · Mar 26, 2008
- 44.T “Peptide Binding to Sheet Silicate and Metal Nanoparticles - Insight from Atomistic Simulation” · MRS Spring Meeting · San Francisco, CA · Mar 25, 2008
- 43.P “Relation between Packing Density and Thermal Transitions of Alkyl Chains on Layered Silicate and Metal Surfaces” · APS March Meeting · New Orleans, LA · Mar 12, 2008
- 42.T “Peptide Binding to Sheet Silicate and Metal Nanoparticles: Insight from Atomistic Simulation” · APS March Meeting · New Orleans, LA · Mar 10, 2008 (R. B. Pandey)

- 41.P “Atomistic simulation of inorganic-biological interfaces and accurate force fields for fcc metals and layered silicates” · Zing Conference on Computational Biophysics with Chemical Accuracy · Jolly Beach Resort · Bolans Village, Antigua · Jan 15, 2008
- 40.T “Self-Assembly of Peptides on Montmorillonite Nanoparticles” · AIChE Annual Meeting · Salt Lake City, UT · Nov 7, 2007
- 39.T “Atomistic Simulation of Peptide Binding to Metal 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 · 93rd Statistical Mechanics Conference · May 16, 2005
- 27.T ”Computer Simulation of the Light-Induced Trans-Cis Isomerization of Azobenzene Grafted Onto Montmorillonite Sheets” · MRS Fall Meeting · Boston, MA · Nov 31, 2005
- 26.P “Modeling of the Photochemical Trans-Cis Isomerization of Azobenzene Confined Between Montmorillonite Sheets” · MRS Fall Meeting · Boston, MA · Nov 31, 2005
- 25.P “Towards Quantitative Modeling of Interface Properties of Organic-Inorganic Hybrid Materials” · AIChE Annual Meeting · Cincinnati, OH · Oct 31, 2005
- 24.T "Calculation of local pressure tensors in systems with many-body interactions" · ACS national meeting · Washington, D. C. · Sep 1, 2005
- 23.T "Free energy of exfoliation between layered silicate sheets" · ACS national meeting · Washington, D. C. · Aug 31, 2005
- 22.T "Towards quantitative modeling of surface properties in inorganic-organic hybrid materials" · ACS national meeting · Washington, D. C. · Aug 31, 2005
- 21.P “Towards Quantitative Modeling of Interface Properties of Organic-Inorganic Hybrid Materials” · ACS National Meeting (AEI) · Washington, D. C. · Aug 29, 2005

- 20.T "Self-assembly of alkylammonium chains on montmorillonite: Effect of chain length, head group structure, and cation exchange capacity" · ACS national meeting Washington, D. C. · Aug 28, 2005
- 19.P "Free Energy of Exfoliation Between Layered Silicate Sheets" · Symposium "Oligomers to Macromolecules in Akron" · University of Akron, OH · Jun 27, 2005 · With R. A. Vaia and B. L. Farmer
- 18.T "Progress in Molecular Modeling of Superplasticizers in 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—7th World Congress of Theoretically Oriented Chemists · Cape Town, South Africa · Jan 19, 2005
- 15.T "Semiempirical Atomistic Simulation of Interactions between Sheets of Layered Silicates" · MRS fall meeting · Boston, MA · Dec 1, 2004
- 14.T "A Semiempirical Energy Model and Atomistic Simulation of Organically Modified Montmorillonite" · MRS fall meeting · Boston, MA · Dec 1, 2004
- 13.T "A Semiempirical Energy Model and Atomistic Simulation of Organically Modified Montmorillonite" · AFRL/ML · Polymer Technology Colloquium · Wright-Patterson AFB Dayton, OH · Nov 24, 2004
- 12.T "Structure and Phase Transitions of Alkylammonium Chains on Mica" · ACS national meeting · Philadelphia, PA · Aug 26, 2004
- 11.P "Atomic Charges for Classical Simulation of Polar Systems" · ACS national meeting · Philadelphia, PA · Aug 23, 2004 · With U. W. Suter
- 10.P "Atomistic Modeling of Organically Modified Mica" · NANO 2004 · Wiesbaden, Germany · Jun 22-26, 2004 · With U. W. Suter
- 9.T "Atomic Charges for Classical Simulations of Polar Systems" · APS march meeting · Montreal, Canada · Mar 26, 2004
- 8.T "A Perylene Chromophore in *n*-alkanes: Modeling Geometries and $\pi \rightarrow \pi^*$ Spectral Shifts Based on Local Electron Density" · APS march meeting · Montreal, Canada · Mar 26, 2004
- 7.P "Atomistic Modeling of Organically Modified Mica" · 20th Annual Meeting of the Swiss User Group Surfaces and Interfaces · Fribourg, Switzerland · Jan 23, 2004 · With U. W. Suter
- 6.T "Molecular Modeling of Superplasticizers in Cementitious Systems: Introductory Steps" · Sika Technology AG · Zürich, Switzerland · Jan 22, 2004
- 5.T "Understanding Materials by Atomistic Simulation?" · Annual Meeting of the Association for the International Chemistry Olympiad · University of Leipzig, Germany · Jan 8, 2004
- 4.P "Structure and Phase Transitions of Alkyl Chains on Mica: Understanding by MD Simulation" · NATO-Advanced Study Institute "Computer Simulation of Surfaces and Interfaces" · Albena Black Sea Resort · Albena, Bulgaria · Sep 9-20, 2002 · with H. J. Castelijns and U. W. Suter
- 3.P "Partial Charges in Polar Solids" · 6th World Congress of Theoretically Oriented Chemists (WATOC) · Lugano, Switzerland · Palazzo dei Congressi · Aug 4-9, 2002 · With U. W. Suter
- 2.T "Dynamics of Alkane Chains on Mica" · ETH Zurich · Department of Materials · Materials Science Seminar · Jul 3, 2002

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

1) Reviewer for Journals: Angewandte Chemie International Edition, Journal of Physical Chemistry, Soft Matter, Macromolecules, Langmuir, Journal of Polymer Science, Polymer, Macromolecular Theory and Simulation, Computational Materials Science, MRS Bulletin, Journal of Materials Research, Mechanics of Time Dependent Materials, Polymer International, Polymer Engineering and Science

2) Reviewer for Proposals: (1) research: AFOSR, ACS-PRF, NSF; (2) books: CRC Press (T&F), Cambridge University Press

3) Editorial supervisory board of Silicon (an international journal)

4) Sessions/symposia organized and in progress:

- Symposium “Simulation of (Bio)Organic-Inorganic Interfaces and Nanostructures Using MD, MC, and Multiscale Approaches” at ACS Fall (2009, D-PMSE & D-COMP)
- Session “Simulation and Theory of Clay Minerals and Interfaces” at XIV. International Clay Conference (2009)
- 3 Sessions “Modeling Composites”, “Multifunctional Composites”, “Properties and Characterization of Nanocomposites” at AIChE (2008)
- Session “Clay Nanomaterials” at the Annual Clay Minerals Society Meeting (2007)

5) Presiding Sessions

ACS Fall 2009, 14th Int. Clay Conference 2009, ICHTM 2009 Kharagpur, APS March Meeting 2008, AIChE 2008, Annual Clay Minerals Society Meeting 2007

Affiliations

- American Chemical Society, member
 - Materials Research Society, member
 - American Physical Society, member
 - Clay Minerals Society, member
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Languages and Hobbies

- German (native), English, Spanish, Russian
- Music (piano), Swimming, Dancing

Teaching Experience

- Advanced Characterization of Functional Polymers · University of Akron Fall 2008
Graduate course
- Nanocomposites · University of Akron Spring 2008
Graduate course (with S. Jana and M. Soucek)
- Engineering Properties of Polymers · University of Akron Spring 2008, 2009
Undergraduate course
- Advanced Functional Polymers · University of Akron Fall 2007
Graduate course
- Simulation of Nanoscale Materials · University of Akron Spring 2007
Graduate course
- Organized Department Seminar · University of Akron Spring 2007
- Assistant Lab Supervisor · ETH Zurich · Switzerland 02/2003 – 03/2003
Undergraduate lab course in polymer science (with Peter Walde)
- Private Teaching 2001 – 2003
Taught several undergraduate students chemistry, physics, and mathematics
- Lecturer · Student Association ETH Zurich 07/2000
Invited to teach an intensive, daily thermodynamics class for 4 weeks with exercises to prepare undergraduate students for their exam needs (1st and 2nd year)
- Teaching Assistant · ETH Zurich 04/2000 – 07/2000
Assistant for an undergraduate environmental chemistry class (with U. Mueller-Herold)
- Teaching Assistant · Leibniz-Institute for Education in the Natural Sciences 1995 – 1998
Germany
Prepared talented 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

Supervising

- Postdocs & visiting Ph.D. scientists (>=3 months): current 1; completed 1
 - PhD students: current 5
 - Master students: current 1; completed 1 (at ETH Zurich 2002)
 - Undergraduate students: current 0; completed 3 (of which 1 at ETH Zurich 2003)
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