

Curriculum Vitae -- Steven Ole Nielsen

Educational History

- Ph.D. 2001
University of Toronto
Department of Chemistry
Thesis Title: Mixed Quantum-Classical Statistical Mechanics and Dynamics
Supervisor: Raymond E. Kapral
- M.Sc. 1998
University of Toronto
Department of Chemistry
Thesis Title: Colouring a Lorentz Gas
Supervisor: Raymond E. Kapral
- B.Sc. 1996
Queen's University (Kingston, Canada)
Mathematics and Chemistry, Honours degree

Employment History

- 2005-present Assistant Professor, Department of Chemistry, University of Texas at Dallas
- 2001-2005 Postdoctoral Fellow under the supervision of Professor Michael L. Klein, Department of Chemistry, University of Pennsylvania
- 1996 Summer research fellowship under the supervision of Tamar Seideman and Albert Stolow, Steacie Institute for Molecular Sciences, National Research Council of Canada (Ottawa, Canada)
- 1995 Summer research fellowship under the supervision of Professor Gren N. Patey, Department of Chemistry, University of British Columbia (Vancouver, Canada)
- 1994 Summer research fellowship under the supervision of Professor David M. Wardlaw, Department of Chemistry, Queen's University (Kingston, Canada)

Recognitions and honors

- 2001-2003 Natural Sciences and Engineering Research Council of Canada (NSERC) Postdoctoral Fellowship
- 1996-2000 NSERC Postgraduate Scholarship
- 1998-2000 Walter C. Sumner Memorial Fellowship (excellence in chemistry, physics or electronics graduate education)
- 1996 Chemistry Medal (top of graduating class, Queen's University)
- 1995 NSERC Undergraduate Summer Scholarship
- 1994 NSERC Undergraduate Summer Scholarship
- 1992-1996 Canada Scholarship for Undergraduate Studies

Professional memberships

American Chemical Society, 2003 – present

Refereed Publications (h-factor = 18; Sum of the Times Cited > 1,000)

37. Steven O. Nielsen, Preston B. Moore, and Bernd Ensing
Adaptive multiscale molecular dynamics of macromolecular fluids
Physical Review Letters **105** 237802 (2010).
36. Russell DeVane, Arben Jusufi, Wataru Shinoda, Chi-cheng Chiu, Steven O. Nielsen, Preston B. Moore, and Michael L. Klein
Parameterization and application of a coarse grained force field for benzene/fullerene interactions with lipids
Journal of Physical Chemistry B **114** 16364-16372 (2010).
35. Steven O. Nielsen, Rosa E. Bulo, Preston B. Moore, and Bernd Ensing
Recent progress in adaptive multiscale molecular dynamics simulations of soft matter
Physical Chemistry Chemical Physics **12** 12401-12414 (2010).
Inside cover article (issue 39)
34. R. J. K. Udayana Ranatunga, Robert J. B. Kalescky, Chi-cheng Chiu, and Steven O. Nielsen
Molecular dynamics simulations of surfactant functionalized nanoparticles in the vicinity of an oil/water interface
Journal of Physical Chemistry C **114** 12151–12157 (2010).
33. Chi-cheng Chiu, Marie C. Maher, Gregg R. Dieckmann, and Steven O. Nielsen
Molecular dynamics study of a carbon nanotube binding reversible cyclic peptide
ACS Nano **4** 2539-2546 (2010).
32. Chi-cheng Chiu, Russell DeVane, Michael L. Klein, Wataru Shinoda, Preston B. Moore, and Steven O. Nielsen
Coarse-grained potential models for phenyl-based molecules: II. Application to fullerenes
Journal of Physical Chemistry B **114** 6394–6400 (2010).
31. Russell DeVane, Michael L. Klein, Chi-cheng Chiu, Steven O. Nielsen, Wataru Shinoda, and Preston B. Moore
Coarse-grained potential models for phenyl-based molecules: I. Parametrization using experimental data
Journal of Physical Chemistry B **114** 6386–6393 (2010).
30. Chi-cheng Chiu, R. J. K. Udayana Ranatunga, David Torres Flores, D. Vladimir Pérez, Preston B. Moore, Wataru Shinoda, and Steven O. Nielsen
A mean field approach for computing solid-liquid surface tension for nanoscale interfaces
Journal of Chemical Physics **132** 054706 (2010).
Selected for the February 15, 2010 issue of Virtual Journal of Nanoscale Science & Technology.
29. Chi-cheng Chiu, Preston B. Moore, Wataru Shinoda, and Steven O. Nielsen
Size-dependent hydrophobic to hydrophilic transition for nanoparticles: A molecular dynamics study
Journal of Chemical Physics **131** 244706 (2009).
Selected for the January 1, 2010 issue of Virtual Journal of Biological Physics Research.

28. Chi-cheng Chiu, Gregg R. Dieckmann, and Steven O. Nielsen
Role of peptide-peptide interactions in stabilizing peptide-wrapped single-walled carbon nanotubes: A molecular dynamics study
Biopolymers: Peptide Science **92** 156-163 (2009).
27. Robert J. B. Kalescky, Wataru Shinoda, Preston B. Moore, and Steven O. Nielsen
Area per ligand as a function of nanoparticle radius: A theoretical and computer simulation
Langmuir **25** 1352-1359 (2009).
26. Uriel Octavio Moreles Vázquez, Wataru Shinoda, Preston B. Moore, Chi-cheng Chiu, and Steven O. Nielsen
Calculating the surface tension between a flat solid and a liquid: A theoretical and computer simulation study of three topologically different methods
Journal of Mathematical Chemistry **45** 161-174 (2009).
25. Chi-cheng Chiu, Gregg R. Dieckmann, and Steven O. Nielsen
Molecular dynamics study of a nanotube-binding amphiphilic helical peptide at different water/hydrophobic interfaces
Journal of Physical Chemistry B **112** 16326-16333 (2008).
24. Bernd Ensing, Steven O. Nielsen, Preston B. Moore, Michael L. Klein, and Michele Parrinello
Energy conservation in adaptive hybrid atomistic/coarse-grain molecular dynamics
Journal of Chemical Theory and Computation **3** 1100-1105 (2007).
23. Ekta Khurana, Steven O. Nielsen, and Michael L. Klein
Gemini surfactants at the air/water interface: A fully atomistic molecular dynamics study
Journal of Physical Chemistry B **110** 22136-22142 (2006).
22. Vanessa Ortiz, Steven O. Nielsen, Michael L. Klein, and Dennis E. Discher
Computer simulation of aqueous block copolymer assemblies: Length scales and methods
Journal of Polymer Science: Part B: Polymer Physics **44** 1907-1918 (2006).
21. Ekta Khurana, Steven O. Nielsen, Bernd Ensing, and Michael L. Klein
Self-assembling cyclic peptides: Molecular dynamics studies of dimers in polar and nonpolar solvents
Journal of Physical Chemistry B **110** 18965-18972 (2006).
20. Carlos F. Lopez, Steven O. Nielsen, Goundla Srinivas, William F. DeGrado, and Michael L. Klein
Probing membrane insertion activity of antimicrobial polymers via coarse-grain molecular dynamics
Journal of Chemical Theory and Computation **2** 649-655 (2006).
19. Goundla Srinivas, Steven O. Nielsen, Preston B. Moore, and Michael L. Klein
Molecular dynamics simulations of surfactant self-organization at a solid-liquid interface
Journal of the American Chemical Society **128** 848-853 (2006).
18. Steven O. Nielsen, Goundla Srinivas, and Michael L. Klein
Incorporating a hydrophobic solid into a coarse grain liquid framework: Graphite in an aqueous amphiphilic environment
Journal of Chemical Physics **123** 124907 (2005).

17. Vanessa Ortiz, Steven O. Nielsen, Dennis E. Discher, Michael L. Klein, Reinhard Lipowsky, and Julian Shillcock
Dissipative particle dynamics simulations of polymersomes
Journal of Physical Chemistry B **109** 17708-17714 (2005).
16. Steve O. Nielsen, Goundla Srinivas, Carlos F. Lopez, and Michael L. Klein
Modeling surfactant adsorption on hydrophobic surfaces
Physical Review Letters **94** 228301 (2005).
Selected for the June 20, 2005 issue of Virtual Journal of Nanoscale Science & Technology.
Selected for the June 15, 2005 issue of Virtual Journal of Biological Physics Research.
15. Vanessa Ortiz, Steven O. Nielsen, Michael L. Klein, and Dennis E. Discher
Unfolding a linker between helical repeats
Journal of Molecular Biology **349** 638-647 (2005).
14. Steve O. Nielsen, Bernd Ensing, Vanessa Ortiz, Preston B. Moore, and Michael L. Klein
Lipid bilayer perturbations around a transmembrane nanotube: A coarse grain molecular dynamics study
Biophysical Journal **88** 3822-3828 (2005).
Cover article (June issue)
13. Carlos F. Lopez, Steve O. Nielsen, Bernd Ensing, Preston B. Moore, and Michael L. Klein
Structure and dynamics of model pore insertion into a membrane
Biophysical Journal **88** 3083-3094 (2005).
Cover article (May issue)
12. Steve O. Nielsen, Carlos F. Lopez, Ivaylo Ivanov, Preston B. Moore, John C. Shelley, and Michael L. Klein
Transmembrane peptide-induced lipid sorting and mechanism of L_{α} -to-inverted phase transition using coarse-grain molecular dynamics
Biophysical Journal **87** 2107-2115 (2004).
11. Goundla Srinivas, John C. Shelley, Steve O. Nielsen, Dennis E. Discher, and Michael L. Klein
Simulation of diblock copolymer self-assembly, using a coarse-grain model
Journal of Physical Chemistry B **108** 8153-8160 (2004).
10. Steve O. Nielsen, Carlos F. Lopez, Goundla Srinivas, and Michael L. Klein
Coarse grain models and the computer simulation of soft materials
Journal of Physics: Condensed Matter **16** R481-R512 (2004).
Cover article (April 21 issue)
9. Carlos F. Lopez, Steve O. Nielsen, Preston B. Moore, and Michael L. Klein
Understanding nature's design for a nanosyringe
Proceedings of the National Academy of Sciences **101** 4431-4434 (2004).
Mentioned on the cover (March 30 issue)
8. Carlos F. Lopez, Steve O. Nielsen, Michael L. Klein, and Preston B. Moore
Hydrogen bonding structure and dynamics of water at the dimyristoylphosphatidylcholine lipid bilayer surface from a molecular dynamics simulation
Journal of Physical Chemistry B **108** 6603-6610 (2004).

7. Steve O. Nielsen, Carlos F. Lopez, Preston B. Moore, John C. Shelley, and Michael L. Klein
Molecular dynamics investigations of lipid Langmuir monolayers using a coarse grain model
Journal of Physical Chemistry B **107** 13911-13917 (2003).
6. Steve O. Nielsen, Carlos F. Lopez, Goundla Srinivas, and Michael L. Klein
A coarse grain model for n-alkanes parameterized from surface tension data
Journal of Chemical Physics **119** 7043-7049 (2003).
5. Carlos F. Lopez, Steve O. Nielsen, Preston B. Moore, John C. Shelley, and Michael L. Klein
Self-assembly of a phospholipid Langmuir monolayer using coarse-grained molecular dynamics simulations
Journal of Physics: Condensed Matter **14** 9431-9444 (2002).
4. Steve Nielsen, Raymond Kapral, and Giovanni Ciccotti
Statistical mechanics of quantum-classical systems
Journal of Chemical Physics **115** 5805-5815 (2001).
3. Steve Nielsen, Raymond Kapral, and Giovanni Ciccotti
Non-adiabatic dynamics in mixed quantum-classical systems
Journal of Statistical Physics **101** 225-242 (2000).
2. Steve Nielsen, Raymond Kapral, and Giovanni Ciccotti
Mixed quantum-classical surface hopping dynamics
Journal of Chemical Physics **112** 6543-6553 (2000).
1. Steve Nielsen and Raymond Kapral
Coloring a Lorentz gas
Journal of Chemical Physics **109** 6460-6468 (1998).

Articles Submitted for Publication

1. R. J. K. U. Ranatunga, C. T. Nguyen, B. A. Wilson, W. Shinoda, and S. O. Nielsen
Molecular dynamics study of nanoparticles and non-ionic surfactant at an oil/water interface
Soft Matter, submitted on 28-Jan-2011, manuscript ID SM-ART-01-2011-005145.

Refereed Book Chapters

3. Bernd Ensing and Steven O. Nielsen
Multiscale molecular dynamics and the reverse mapping problem
In **Trends in Computational Nanomechanics (Challenges and Advances in Computational Chemistry and Physics, Volume 9)**, pages 25-60
T. Dumitrica (editor)
Springer (2010)
ISBN: 978-1-4020-9784-3

2. Steven O. Nielsen, Bernd Ensing, Preston B. Moore, and Michael L. Klein
Coarse grain to atomistic mapping algorithm: A tool for multiscale simulations
In **Multiscale Simulation Methods for Nanomaterials**, pages 73-88
R.B. Ross and S. Mohanty (editors)
Wiley (2008)
ISBN: 0470105283

1. Steve O. Nielsen and Michael L. Klein
A coarse grain model for lipid monolayer and bilayer studies
In **Bridging the Time Scales: Molecular Simulations for the Next Decade (Lecture Notes in Physics, 605)**, pages 27-63
P. Nielaba, M. Mareschal and G. Ciccotti (editors)
Springer (2002)
ISBN: 3540443177

Book Chapters Accepted for Publication

1. R. J. K. Udayana Ranatunga, Chuong T. Nguyen, Chi-cheng Chiu, Wataru Shinoda, and Steven O. Nielsen
Molecular Dynamics Simulations of Nanoparticles and Surfactants at Oil/Water Interfaces
In **Amphiphiles: Molecular Assembly and Applications (ACS Books Symposium Series)**
R. Nagarajan (editor)
Date Submitted: 24-Jun-2010
American Chemical Society
Submitted Manuscript ID: bk-2010-00323a
Date Accepted for Publication: 08-Feb-2011

Invited and Refereed Conference Presentations

- 2011 15th SRC/SEMATECH Engineering Research Center for Environmentally Benign Semiconductor Manufacturing Review Meeting (invited talk)
Predicting, testing, and neutralizing nanoparticle toxicity
Tuscon, AZ

- 2011 Young Investigator American Chemical Society DFW Local Section Meeting (invited talk)
Recent progress in adaptive multiscale molecular dynamics simulations of soft matter
Dallas, TX

- 2010 Southwest Theoretical Chemistry Conference (SWTCC 2010) (contributed talk)
Recent progress in adaptive multiscale molecular dynamics simulations of soft matter
Denton, TX

- 2010 240th American Chemical Society National Meeting (contributed talk)
Effect of spherical fullerenes on pulmonary lipid monolayers: Molecular dynamics simulations
Boston, MA

- 2010 240th American Chemical Society National Meeting (contributed talk)
Molecular dynamics simulations of nanoparticles and surfactants at oil/water interfaces: Chemisorption vs. physisorption
Boston, MA

- 2010 17th Canadian Symposium on Theoretical Chemistry (invited talk)
Adaptive multiscale molecular dynamics of macromolecular fluids
Edmonton, Canada
- 2010 93rd Canadian Society for Chemistry Conference (invited talk)
Molecular dynamics simulation of nanoscale interfaces: From simple liquids to biological systems
Toronto, Canada
- 2010 239th American Chemical Society National Meeting (contributed talk)
Molecular dynamics study of a reversible nanotube binding cyclic peptide
San Francisco, CA
- 2010 239th American Chemical Society National Meeting (contributed talk)
Molecular dynamics simulations of nanoparticles functionalized with amphiphilic ligands at oil/water interfaces
San Francisco, CA
- 2010 14th SRC/SEMATECH Engineering Research Center for Environmentally Benign Semiconductor Manufacturing Review Meeting (invited talk)
Predicting, testing, and neutralizing nanoparticle toxicity
Tuscon, AZ
- 2009 13th SRC/SEMATECH Engineering Research Center for Environmentally Benign Semiconductor Manufacturing Review Meeting (invited talk)
Predicting, testing, and neutralizing nanoparticle toxicity
Tuscon, AZ
- 2008 Escuela de Modelación y Métodos Numéricos: Supercómputo y Aplicaciones (invited talk)
Young's equation: What's wrong at the nanoscale and how to fix it
Centro de Investigación en Matemáticas, Guanajuato, Mexico
- 2008 236th American Chemical Society National Meeting (contributed talk)
Nanoparticle localization energy at the oil/water interface: Effect of the deformable organic ligand coating
Philadelphia, PA
- 2008 235th American Chemical Society National Meeting (contributed talk)
Young's equation: What's wrong at the nanoscale and how to fix it
New Orleans, LA
- 2007 Gordon Conference on the Chemistry and Physics of Liquids (contributed poster)
Nanoparticles composed of macroscopically hydrophilic material become hydrophobic on the nanometer length scale
Holderness School, NH
- 2007 Lattices and Trajectories: A Symposium of Mathematical Chemistry in Honour of Ray Kapral and Stu Whittington (contributed talk)
Nanoparticles composed of macroscopically hydrophilic material become hydrophobic on the nanometer length scale
Toronto, Canada

- 2006 US-Ireland NSF Nanotechnology Workshop (invited poster)
Self-assembly in biological and materials systems: Computer modeling at the mesoscopic level
Belfast, North Ireland
- 2006 50th Biophysical Society Annual Meeting (contributed poster)
Transmembrane nanotube studies using coarse grain molecular dynamics: Bilayer response to hydrophobic mismatch
Salt Lake City, UT
- 2005 Multiscale modeling in soft matter and bio-physics (invited talk)
Coarse grained to atomistic mapping algorithm: A tool for multiscale simulations
Institute for Pure and Applied Mathematics, UCLA
- 2005 230th American Chemical Society National Meeting (invited talk)
Coarse grained to atomistic mapping algorithm: A tool for multiscale simulations
Washington, DC
- 2004 Emerging Challenges in Membrane Biophysics (invited talk)
Coarse grain molecular dynamics study of interactions between transmembrane nanotubes
Sun Valley, ID
- 2004 228th American Chemical Society National Meeting (contributed talk)
Coarse grain molecular dynamics study of interactions between transmembrane nanotubes
Philadelphia, PA
- 2003 Gordon Conference on the Chemistry and Physics of Liquids (poster award talk)
Coarse grain molecular dynamics simulations of membranes
Holderness School, NH
- 2003 226th American Chemical Society National Meeting (contributed talk)
Mechanism of peptide-induced lamellar to inverted hexagonal phase transition in phospholipid systems using coarse grain molecular dynamics
New York, NY
- 1999 82nd Canadian Society for Chemistry Conference (invited talk)
Mixed quantum-classical dynamics
Toronto, Canada

Invited Seminars

- 2011 *Adaptive multiscale molecular dynamics of macromolecular fluids*
LONI Institute/LA-SiGMA, Louisiana State University (Baton Rouge, LA)
- 2009 *Nanoparticles from a soft matter viewpoint: Surface tension and ligand coating studied using computer simulation methods*
Research Institute for Computational Sciences, National Institute of Advanced Industrial Science and Technology (AIST, Japan)
- 2009 *Nanoparticles from a soft matter viewpoint: Surface tension and ligand coating studied using computer simulation methods*
Department of Chemistry, Texas Christian University (Fort Worth, TX)

- 2009 *Nanoparticles from a soft matter viewpoint: Surface tension and ligand coating studied using computer simulation methods*
Department of Physics, University of Texas at Dallas
- 2008 *Young's equation: What's wrong at the nanoscale and how to fix it*
John van Geuns Foundation Invited Talk
Van't Hoff Institute for Molecular Sciences, University of Amsterdam
- 2008 *Young's equation: What's wrong at the nanoscale and how to fix it*
Department of Chemistry, University of Guanajuato, Mexico
- 2007 *Quantifying the surfactant coverage of nanoparticles by molecular dynamics simulation: The physisorbed versus chemisorbed cases*
Research Institute for Computational Sciences, National Institute of Advanced Industrial Science and Technology (AIST, Japan)
- 2005 *Coarse grained strategies for aqueous surfactant adsorption onto hydrophobic solids: Slabs, nanotubes, and quantum dots*
Institute for Theoretical Chemistry, University of Texas at Austin
- 2005 *Membrane protein stability and aggregation*
Chemical and Biomolecular Engineering, Johns Hopkins University
- 2005 *Membrane protein stability and aggregation*
Department of Chemistry, University of British Columbia (Vancouver, Canada)
- 2005 *Membrane protein stability and aggregation*
Department of Chemistry, University of Texas at Dallas
- 2004 *Modeling the solubilization of carbon nanotubes in aqueous surfactant*
Theory Division, Max Planck Institute of Colloids and Interfaces (Potsdam, Germany)
- 2004 *Modeling surfactant solubilization of carbon nanotubes: materials and biological applications*
Physics Department, McGill University (Montreal, Canada)
- 2003 *Coarse grain studies of aqueous amphiphilic systems: Membrane-peptide interactions and surfactant coverage of graphite sheets*
Computational Biophysics Section, National Institutes of Health (Bethesda, MD)

External Funding

Proposals submitted:

1. Molecular details on the cooperative action of amphiphilic peptides as membrane active antimicrobials and as dispersing agents for carbon nanotubes
S.O. Nielsen (PI)
The Camille and Henry Dreyfus Foundation New Faculty Award \$50,000 (2005, not funded)

2. S.O. Nielsen (PI)
Sloan Research Fellowship \$45,000 (2006, not funded)
3. **Surfactant adsorption and self-assembly at solid/liquid interfaces**
S.O. Nielsen (PI)
American Chemistry Society Petroleum Research Fund 'Type G' \$40,000 (2006, funded)
4. Surfactant adsorption and self-assembly at solid/liquid interfaces
S.O. Nielsen (PI)
American Chemistry Society Petroleum Research Fund SUMR Supplement \$3,700 (2006, not funded)
5. Computer simulation studies of the aggregation and biocompatibility of surfactant encapsulated quantum dots
S.O. Nielsen (PI)
Welch Foundation \$150,000 (2006, not funded)
6. Non-invasive mapping of tissue redox status using PARACEST MRI agents designed from quantum chemical principles
S.O. Nielsen (co-PI) and Z. Kovacs (co-PI)
UTD/UTSW Joint Venture Grants for Collaborative Research \$40,000 (2006, not funded)
7. Self-assembly of 3D photonic quasicrystals from colloidal nanoparticles: A computer simulation study
S.O. Nielsen (PI)
Welch Foundation \$150,000 (2007, not funded)
8. **Non-invasive mapping of tissue redox status using PARACEST MRI agents designed from quantum chemical principles**
S.O. Nielsen (PI)
Texas Advanced Computing Center (2007, 50 000 hours of supercomputer time awarded)
9. Noncovalent functionalization of carbon nanotubes using designed polypeptides
G.R. Dieckmann (PI), A.B. Dalton (co-PI), C. Gilpin (co-PI), I.H. Musselman (co-PI), S.O. Nielsen (co-PI)
NSF \$1,497,294 (2007, not funded)
10. Microscopy and spectroscopy studies of the electronic properties of peptide/carbon nanotube composites
I.H. Musselman (PI), A.B. Dalton (co-PI), G.R. Dieckmann (co-PI), S.O. Nielsen (co-PI)
NSF \$1,107,593 (2007, not funded)
11. S.O. Nielsen (PI)
Sloan Research Fellowship \$45,000 (2007, not funded)
12. Non-invasive mapping of tissue redox status using MRI agents designed from quantum chemistry
S.O. Nielsen (PI), Z. Kovacs (co-PI)
Norman Hackerman Advanced Research Program pre-proposal (2007, not accepted)
13. Surfactant adsorption and self-assembly at solid/liquid interfaces
S.O. Nielsen (PI)
Research Corporation Cottrell Scholar Award \$100,000 (2007, not funded)

14. GOALI: Fundamentals of plasma-wall interactions in fluorocarbon plasmas
M.J. Goeckner (PI), A. Balakrishna (co-PI), S.O. Nielsen (co-PI), L.J. Overzet (co-PI)
NSF \$761,338 (2008, not funded)
15. Theory of nanoparticle self-assembly at oil/water interfaces
S.O. Nielsen (PI), P.B. Moore (co-PI), W. Shinoda (co-PI)
NSF \$550,044 (2008, not funded)
16. **Noncovalent functionalization of carbon nanotubes using designed polypeptides**
S.O. Nielsen (PI)
Texas Advanced Computing Center (2008, 50 000 hours of supercomputer time awarded)
17. Reversible cyclic peptides for carbon nanotube functionalization
G.R. Dieckmann (PI), C. Gilpin (co-PI), I.H. Musselman (co-PI), S.O. Nielsen (co-PI)
NSF \$552,813 (2008, not funded)
18. CAREER: A theoretical and computer simulation approach to control inorganic/organic interfaces in materials science
S.O. Nielsen (PI)
NSF \$426,427 (2008, not funded)
19. Theory and computer simulations of nanoparticle-organic interfaces in materials science
S.O. Nielsen (PI), P.B. Moore (co-PI), W. Shinoda (co-PI)
NSF \$262,945 (2008, not funded)
20. Microscopy and spectroscopy studies of the electronic properties of peptide/carbon nanotube composites
I.H. Musselman (PI), G.R. Dieckmann (co-PI), S.O. Nielsen (co-PI)
NSF \$450,125 (2008, not funded)
21. Developing high resolution imaging methodologies for soft matter-functionalized nanomaterials
I.H. Musselman (PI), G.R. Dieckmann (co-PI), C. Gopin (co-PI), S.O. Nielsen (co-PI)
NSF \$495,937 (2008, not funded)
22. Molecular dynamics simulations of nanoparticles coated with surface-bound ligands
S.O. Nielsen (PI), P.B. Moore (co-PI), W. Shinoda (co-PI)
NSF \$262,945 (2008, not funded)
23. S.O. Nielsen (PI)
Sloan Research Fellowship \$50,000 (2008, not funded)
24. Novel selective separation of metallic and semiconducting SWNTs (single-walled carbon nanotubes)
D.J Yang (PI), S.O. Nielsen (co-PI)
Air Force AFOSR \$360,000 (2008, not funded)
25. Measuring surface tension: A computer simulation study
S.O. Nielsen (PI)
Welch Foundation \$150,000 (2008, not funded)

26. Energy storage research
K.J. Cho (PI), S.O. Nielsen (one of 18 co-PIs)
DOE EFRC \$14,892,269 (2008, not funded)
27. **Predicting, testing, and neutralizing nanoparticle toxicity**
S.O. Nielsen (PI), R.K. Draper (co-PI), P. Pantano (co-PI), I.H. Musselman (co-PI),
G.R. Dieckmann (co-PI)
SRC/SEMATECH Semiconductor Research Corporation Global Research
Collaboration \$770,125 (2008, funded)
28. Controlled patterning of carbon nanotube surfaces using designed peptides
G.R. Dieckmann (PI), C. Gilpin (co-PI), I.H. Musselman (co-PI), S.O. Nielsen (co-PI)
NSF \$ 501,182 (2009, not funded)
29. CAREER: Use of simple geometrical objects in molecular dynamics simulations
S.O. Nielsen (PI)
NSF \$ 408,121 (2009, not funded)
30. Molecular dynamics simulations of functionalized nanoparticles at liquid/liquid interfaces
P.B. Moore (PI), S.O. Nielsen (co-PI)
NSF \$ 397,870 (2009, not funded)
31. Electrical properties of peptide/nanotube composites
I.H. Musselman (PI), G.R. Dieckmann (co-PI), M. P. in het Panhuis (co-PI),
S.O. Nielsen (co-PI)
NSF \$ 481,938 (2009, not funded)
32. Pushing the information limit in electron tomography: The way forward
G.R. Dieckmann (PI), I.H. Musselman (co-PI), C. Gilpin (co-PI), S.O. Nielsen (co-PI)
NIH Challenge Grant \$ 933,936 (2009, not funded)
33. Enhancing student engagement in large classes: Using peer instruction with personal response systems
R.C. Hilborn (PI), R. Blackburn (co-PI), G.R. Dieckmann (co-PI), M. Ishak-Boushaki (co-PI), S.O. Nielsen (co-PI)
University of Texas System Transforming Undergraduate Education (TUE), \$246,488
(2009, not funded)
34. Surface and line tension at the nanoscale: New strategies to calculate two- and one-dimensional quantities by molecular simulation
S.O. Nielsen (PI)
Welch Foundation \$150,000 (2009, not funded)
35. Nanomaterial behavior at fluid interfaces: The role of surface energy
S.O. Nielsen (PI)
Welch Foundation \$100,000 (2010, not funded)
36. CAREER: Use of simple geometrical objects in molecular dynamics simulations
S.O. Nielsen (PI)
NSF \$ 440,273 (2010, not funded)
37. Controlled patterning of carbon nanotube surfaces using designed peptides
G.R. Dieckmann (PI), C. Gilpin (co-PI), I.H. Musselman (co-PI), S.O. Nielsen (co-PI)
NSF \$ 826,391 (2010, not funded)

38. Electrical properties of peptide/nanotube composites
I.H. Musselman (PI), G.R. Dieckmann (co-PI), M. P. in het Panhuis (co-PI),
S.O. Nielsen (co-PI)
NSF \$ 740,988 (2010, not funded)
39. GOALI: Fundamental molecular understanding of hydrophobic materials produced by Y-
Carbon
P.B. Moore (PI), R. Dash (co-PI), S.O. Nielsen (co-PI)
NSF \$ 412,477 (2010, pending)
40. Adaptive multiscale molecular dynamics simulations: Creating the new paradigm for
molecular modeling
S.O. Nielsen (PI)
Welch Foundation \$100,000 (2011, pending)
41. Free energy of nano-interfaces
S.O. Nielsen (PI)
Camille Dreyfus Teacher-Scholar Award \$75,000 (2011, pending)
42. Molecular Recognition in Triazine Dendrimers
E.E. Simanek (PI), O. Annunziata (co-PI), G. Pavan (co-PI), S.O. Nielsen (co-PI)
NIH R01 Competitive Renewal, co-PI Nielsen's portion of the budget is \$340,000 in direct
costs, \$520,000 including indirect (2011, pending)

Grants awarded:

1. Investigator: S. O. Nielsen (PI)
Title: *Surfactant adsorption and self-assembly at solid/liquid interfaces*
Source: American Chemical Society Petroleum Research Fund
Amount: \$40,000
Period: 01/01/07 – 08/31/09
2. Investigator: S. O. Nielsen (PI)
Title: *Non-invasive mapping of tissue redox status using PARACEST MRI agents
designed from quantum chemical principles*
Source: Texas Advanced Computing Center
Amount: 50 000 hours of supercomputer time
Period: 01/01/07 – 08/31/10
3. Investigator: S. O. Nielsen (PI)
Title: *Noncovalent functionalization of carbon nanotubes using designed
polypeptides*
Source: Texas Advanced Computing Center
Amount: 50 000 hours of supercomputer time
Period: 01/01/08 – 08/31/10
4. Investigators: S.O. Nielsen (PI), R.K. Draper (co-PI), P. Pantano (co-PI), I.H. Musselman
(co-PI), G.R. Dieckmann (co-PI)
Title: *Predicting, testing, and neutralizing nanoparticle toxicity*
Source: SRC/SEMATECH Semiconductor Research Corporation Global Research
Collaboration

Amount: Year 1: \$120,000 from SRC. In addition, \$45,000 of matching funds from the NS&M Dean's Office and \$20,000 of matching funds from the Office of the Vice President for Research (04/01/09 – 03/31/10)
Year 2: \$120,000 from SRC. In addition, \$20,000 of matching funds from the Office of the Vice President for Research (04/01/10 – 03/31/11)
Year 3: TBA
Period: 04/01/09 - 03/31/12

Teaching: Student advisement

Doctoral

2. R. J. K. Udayana Ranatunga, UTD
Nanoparticle stability and organization at oil/water interfaces
Fall 2009 – present
1. Chi-cheng Chiu, UTD
Molecular dynamics simulation of nanoscale interfaces: From simple liquids to biological systems
Fall 2007 – Spring 2010
Ph.D. degree awarded Spring 2010

Masters

4. R. J. K. Udayana Ranatunga, UTD
Molecular dynamics study of diethyleneglycol-monododecyl ether functionalized nanoparticles at an oil-water interface
Spring 2008 – Fall 2009
Masters degree awarded Fall 2009
3. Robert J. B. Kalescky, UTD
Area per ligand as a function of nanoparticle radius: A theoretical and computer simulation approach
Fall 2007 – Spring 2009
Masters degree awarded Spring 2009
2. Chi-cheng Chiu, UTD
Conformational study of nano-1 peptide at the water / carbon nanotube interface using molecular dynamics simulations
Fall 2005 – Fall 2007
Masters degree awarded Fall 2007
1. Georgia L. Serfling, UTD
Incorporating explicit electrostatic screening at the coarse grain level
Fall 2005 – Spring 2007, candidate withdrew

Undergraduate

11. Assefa D. Siraro, UTD
Molecular dynamics simulation of nanoparticles and surfactants at interfaces
Spring 2011 – present
UTD Research Internship

10. Blake A. Wilson, UT Tyler
Molecular dynamics simulation of nanoparticles and surfactants at interfaces
Summer 2010
Louis Stokes Alliances for Minority Participation (LSAMP) Program Internship
9. Srilakshmi Chetlur, UTD
Thermodynamics of MABA-RC5-Cys – carbon nanotube interaction
Summer 2010 – Fall 2010
UTD Research Internship
8. Suleyman B. Tufa, UTD
Interaction of nanoparticles at oil/water interfaces
Spring 2010
UTD Research Internship
7. Chuong T. Nguyen, UTD
Mechanical strength of colloidosomes
Fall 2009 – Spring 2010
UTD Research Internship
6. David Torres Flores, Centro de Investigación en Matemáticas (CIMAT), Guanajuato, Mexico
A mean field approach for computing solid-liquid surface tension for nanoscale interfaces
Summer 2009
UTD-Mexico Exchange Program
5. Min Zhou, UTD
Peptide/nanotube and peptide/peptide binding strengths
Fall 2007 – Spring 2008
UTD Research Internship
4. Marie C. Maher, UTD
Thermodynamics of RC5-cys interaction with carbon nanotubes
Fall 2007 – Summer 2008
UTD Research Internship
3. Uriel Octavio Moreles Vázquez, Centro de Investigación en Matemáticas (CIMAT), Guanajuato, Mexico
Calculating the surface tension between a flat solid and a liquid: A theoretical and computer simulation study of three topologically different methods
Summer 2007
UTD-Mexico Exchange Program
2. Darren C. Ware, UTD
Crossing angle dependence of nano-1 on carbon nanotube diameter and chirality
Summer 2007 – Fall 2007
UTD Research Internship
1. David O. Birdwell, UTD
A molecular dynamics study of the nano-1 peptide at a graphite/water and graphite/methanol interface using the CHARMM forcefield
Fall 2006 – Spring 2007
UTD Research Internship

High School

3. Jieun Lim, Houston
The study of reversible cyclic peptide stacking on single walled carbon nanotubes using molecular dynamics simulations
2008 Welch Summer Scholar
2. Chris Q. Li, Houston
The importance of phenylalanine at the a/d positions in the designed alpha-helical peptide nano-1: Solubilization of single wall carbon nanotubes studied using molecular dynamics computer simulations
2007 Welch Summer Scholar
1. Jenny J. Zhou, Houston
The effect of surface geometry on the interaction between graphene and the peptide nano-1: Results from computer simulations
2006 Welch Summer Scholar

M.S. and Ph.D. Thesis Committee Member (for UTD students other than my own)

13. Yang Xi
Advisor: A. D. Sherry
2009 – present
12. Harsha D. Magurudeniya
Advisor: M. C. Stefan
2009 – present
11. David K. Bushdiecker II
Advisor: I. M. Musselman
2009 – present
10. Chen Zhou
Advisor: J. Zheng
2008 – present
9. Leila C. R. Fidelino
Advisor: A. D. Sherry
2008 – present
8. Hien Nguyen
Advisor: M. C. Stefan
2008 – present
7. Pathum Panapitiya
Advisor: J. W. Sibert
2008 – present
6. Yixun Xing
Advisor: A. D. Sherry
2008 – present

5. Anton Klimenko
Advisor: G. R. Dieckmann
2008 – present
4. Dinushi R. Samarajeewa
Advisor: I. H. Musselman
2007 – present
3. Fadwa H. Anka
Advisor: J. W. Sibert
2007 – 2009 (M.S. awarded spring 2009)
2. Jane H. Nguyen
Advisor: G. R. Dieckmann
2006 – present
1. Mohamed Sakrout
Advisor: J.-M. Ahn
2005 – present

Teaching: Classroom Teaching

<u>Semester</u>	<u>Prefix</u>	<u>Number</u>	<u>Course Name</u>	<u>Enrollment</u>
2011 Spring	Chem	6V19	Topics in Physical Chemistry	8
2011 Spring	Chem	3322	Physical Chemistry II	43
2010 Fall	Chem	5314	Advanced Physical Chemistry	16
2010 Fall	Chem	1111-107	General Chemistry I Lab	29
2010 Fall	Chem	1111-108	General Chemistry I Lab	30
2010 Spring	Chem	3322	Physical Chemistry II	53
2009 Fall	Chem	5314	Advanced Physical Chemistry	11
2009 Spring	Chem	3322	Physical Chemistry II	31
2009 Spring	Chem	6V19	Topics in Physical Chemistry	8
2008 Fall	Chem	5314	Advanced Physical Chemistry	19
2008 Spring	Chem	3322	Physical Chemistry II	35
2007 Fall	Chem	1311	General Chemistry I	119
2007 Fall	Chem	5314	Advanced Physical Chemistry	8
2007 Spring	Chem	3322	Physical Chemistry II	35
2007 Spring	Chem	6361	Physical Biochemistry	6
2006 Fall	Chem	1311	General Chemistry I	167
2006 Fall	Chem	5314	Advanced Physical Chemistry	13
2006 Spring	Chem	3411	Physical Chemistry I	15
2006 Spring	Chem	6361	Physical Biochemistry	8
2006 Spring	Chem	6V39	Topics in Organic Chemistry	2
2006 Spring	Chem	4V01	Topics in Organic Chemistry	2
2006 Spring	Chem	1112-103	General Chemistry II Lab	36
2006 Spring	Chem	1112-104	General Chemistry II Lab	34
2005 Fall	Chem	5314	Advanced Physical Chemistry	16

Professional and University Citizenship and Service

Reviewer

Journals

2010	Journal of Computational Chemistry
2010	Nanoscale
2010	Physical Chemistry Chemical Physics
2010	Proceedings of the National Academy of Sciences of the USA
2009 – present	ACS Nano
2009 – present	Journal of the American Chemistry Society
2008 – present	Langmuir
2008 – present	Macromolecules
2007 – present	Journal of Physical Chemistry
2005 – present	Physical Review Letters
2004 – present	Biophysical Journal
2003 – present	Journal of Chemical Physics

Funding Agencies

2010	Biotechnology and Biological Sciences Research Council (UK)
2010	Royal Society of New Zealand
2008 – present	Department of Energy
2006 – present	National Science Foundation

Editorial Board Member

2010 – term ending Dec. 2012 Experimental Biology and Medicine

Departmental Activities and Committees

2010 – present	Graduate admissions committee chair
2010 – present	Chemistry webpage manager
2010 – present	Curriculum alignment committee member
2008 – present	Graduate admissions committee member
2007 – 2008	Seminar coordinator
2007	Search committee member for faculty hire in analytical chemistry

School Activities and Committees

2009 -- 2010	Search committee member for UTD Physics Department faculty hire in soft matter physics
2009	Keynote speaker at 2009 UTD Chem/Bio Research Symposium

University Activities and Committees

2007 – present Member of Academic Senate

Community Service

2011	Judge, Dallas Regional Science & Engineering Fair
2010	Participant, “Ballet Stuffing” of envelopes for mailing to the 1400+ local section members for the 2011 ACS DFW local section officer elections
2010	Mentor, Louis Stokes Alliances for Minority Participation (LSAMP) program

2010	Organizer, 43rd Annual American Chemical Society Dallas-Fort Worth Local Section 'Meeting-in-Miniature'
2005 – present	Session Chair, American Chemical Society National Meetings
2007	Member, Chemistry Organizing Committee, Dallas Regional Science Olympiad