

# Peter T. Cummings

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## Education

University of Melbourne, Australia	Mathematics (Stat. Mech.)	Ph.D., 1980
University of Newcastle, Australia	Mathematics (1st class Honors)	B.S., University Medal, 1976

## Research Interests

Molecular modeling of fluid and amorphous systems using the techniques of integral equations (both analytic and numerical solutions), perturbation theory and computer simulation. Application of massively parallel computers to molecular simulation of complex systems, such as polymer blends, alkane chain fluids, and high-temperature high-pressure aqueous solutions. Computer-aided process design and optimization. Mathematical modeling of biological systems. Computational and theoretical nanoscience.

## Professional Experience

2002–p	John R. Hall Professor of Chemical Engineering, Vanderbilt University, Nashville
2007–p	Principal Scientist, Center for Nanophase Materials, ORNL
2006–p	Joint Faculty Appointee, Vanderbilt University/ORNL
2002–2006	Distinguished Visiting Scientist, Chemical Sciences Division, ORNL
2002–2007	Founder and Director, Nanomaterials Theory Institute, Center for Nanophase Materials Sciences, ORNL
2001–2002	Distinguished Scientist, Chemical Sciences Division, ORNL
1994–2001	Distinguished Scientist, Chemical Technology Division, ORNL
2002–2003	Adjunct Professor of Chemical Engineering, University of Tennessee, Knoxville
1994–2002	Distinguished Professor of Chemical Engineering, Chemistry and Computer Science, University of Tennessee, Knoxville
1983–1993	Assistant ('83-'87), Associate ('87-'91) and Full ('91-'93) Professor, Chemical Engineering, University of Virginia, Charlottesville

## Professional and Synergistic Activities

1996–2007	Founding chair: Molecular Modeling Task Force of CACHE educational foundation ( <a href="http://www.cache.org">www.cache.org</a> )
2000–p	Chair: FOMMS 2000 conference and founder of the FOMMS conference series (every three years since 2000)
2003–p	Member: Basic Energy Advisory Committee (BESAC)
1999–2000	Panelist: inter-agency (NSF, DOE, NIST, DOD, NIH)
1989–1991	Member: National Steering Committee, Federal Demonstration Project

## Honors and Awards

2012	Yeram S. Touloukian Award, American Society of Mechanical Engineers
2010	Founders Award, American Institute of Chemical Engineers
2009	Fellow, American Institute of Chemical Engineers
2007	Fellow, American Association for the Advancement of Science (AAAS); Vanderbilt University Chancellor's Award for Research; American Institute of Chemical Engineers Nanoscale Science and Engineering Forum Award
2005	Fellow, American Physical Society
1999	Lockheed-Martin Research Achievement Award for sustained research accomplishment
1998	Alpha Chi Sigma Award from the American Institute of Chemical Engineers (recognizing most outstanding research achievement over the previous decade)
1997	Lockheed-Martin Technical Achievement Award for Publications
1996	University of Virginia President and Board of Visitors Prize for research in the life science
2011–p	Associate Editor, <i>AIChE Journal</i>

2000–2011	Editor, <i>Fluid Phase Equilibria</i>
1997–2006	Advisory Board, <i>Molecular Physics</i>
2002–p	Editorial Board, <i>Journal of Chemical Thermodynamics</i>
2003–p	Editorial Board, <i>Journal of Theoretical and Computational Nanoscience</i>
2006–2011	Editorial Board, <i>Molecular Physics</i>

**Selected Peer-Review Publications:** (Author of >330 refereed journal publications)

- Simpson, M. L. and Cummings, P. T., “Fluctuations and Correlations in Physical and Biological Nanosystems: The Tale Is in the Tails,” *ACS NANO* **5** (2011) 2425-2432 [*Perspective Article*]
- Iacovella, C. R., French, W.R., Cook, B.G., Kent, P.R.C., and Cummings, P.T., "Role of Polytetrahedral Structures in the Elongation and Rupture of Gold Nanowires," *ACS Nano*, **5**, 10065–10073 (2011).
- Feng, G. Cummings, P. T., "Supercapacitor Capacitance Exhibits Oscillatory Behavior as a Function of Nanopore Size," *Journal of Physical Chemistry Letters*, **2**, 2859-2864 (2011).
- Docherty, H. and Cummings P. T., “Direct evidence for fluid-solid transition of nanoconfined fluids,” *Soft Matter* **6** (2010) 1640-1643.
- Pu, Q., Leng, Y., and Cummings, P. T., “Rate-Dependent Energy Release Mechanism of Gold Nanowires under Elongation,” *Journal of the American Chemical Society*, **130** (2008), 17907–17912.
- “Phase Transformations during Sintering of Titania Nanoparticles,” V. N. Koparde and P. T. Cummings, *ACS Nano* **2**, 162–1624 (2008).
- “Electrophoresis of ss-DNA through Nanoelectrode Gaps from Molecular Dynamics: Impact of Gap Width and Chain Length,” C. M. Payne, X.-C. Zhao, and P. T. Cummings, *J. Phys. Chem. B* **112**, 12851–12858 (2008).
- “Coarse-Grained Force Field for Simulating Polymer-Tethered Silsesquioxane Self-Assembly in Solution,” E. R. Chan, A. Striolo, C. McCabe, P. T. Cummings, and S. C. Glotzer, *J. Chem. Phys.* **127**, Art. No. 114102 (2007).
- “Molecular Dynamics Simulations of Stretched Gold Nanowires: The Relative Utility of Different Semi-Empirical Potentials,” Q. Pu, Y. S. Leng, L. Tsetseris, H. S. Park, S. T. Pantelides and P. T. Cummings, *J. Chem. Phys.* **126**, 144707 (2007).
- “Water Adsorption in Carbon-Slit Nanopores,” A. Striolo, A. A. Chialvo, P. T. Cummings and K. E. Gubbins, *Langmuir* **19**, 8583–8591 (2003).
- “Tumor Evolution by Microenvironment Selection,” A. R. A. Anderson, A. M. Weaver, P. T. Cummings, and V. Quaranta, *Cell* **127**, 905–915 (2006).
- “Self-Assembly in a Dichain Surfactant/Water/Carbon Dioxide System via Molecular Simulation. 1. Structural Properties of Surfactant Aggregates,” S. Salaniwal, S. T. Cui, P. T. Cummings and H. D. Cochran, *Langmuir* **17**, 1773–1783 (2001).
- “Molecular Dynamics Study of Water Adsorption on TiO<sub>2</sub> Nanoparticles,” V. N. Koparde and P. T. Cummings, *J. Phys. Chem. C* **111**, 6920–6926 (2007).

**Collaborators Outside ORNL During Past Two Years:** A. Badura, PSU; J. Bedzyk, Argonne National Laboratory; J. Bernholc, NCSU; L. Cheng, Argonne National Laboratory; J. Dongarra, U. Tenn; P. Fenter, Argonne National Laboratory; A. Galindo, Imperial College-London; S.C. Glotzer, Institute for Condensed Matter Fundamentals-Ukraine; K.E. Gubbins, NCSU; J. Kieffer, U. Mich.; Kalyuzhnyi, Y.V., Institute for Condensed Matter Fundamentals- Ukraine; D.A. Kofke, SUNY-Buffalo; J. Kubicki, PSU; S. H. Lee, Kyungsoong University-South Korea; S. N. Lvov, PSU; M. L. Machesky, Illinois Water Survey; M. K. Ridley, Texas Tech; N.C. Sturchio, Argonne National Laboratory; Z. Zhang, Argonne National Laboratory;

**Graduate and Postdoctoral Advisors:** E. R. Smith, Mathematics, La Trobe University, Australia (Ph.D. advisor); C. G. Gray, Physics, Guelph University, Canada (Postdoctoral Advisor, 1980); G. Stell, Chemistry, SUNY at Stony Brook (Postdoctoral Advisor, 1981–83)

**Thesis Advisor and Postgraduate-Scholar Sponsor (last 2 years):**

**Graduate Students** (29 M.S., 30 Ph.D. total): Christina Smith (Washington Group), Zhi Tao (Sriya Innovations), Patrick Redmill (Bryan Engineering), Qing Pu (Brewer Science), Peter Dyer (Industrial Research Ltd, NZ), Alka Potdar (Cleveland Clinics), Will French (current), Li Wan (current), Song Li (current), Siladitya Murkherjee (current), Jana Black (current)

**Postdoctoral Scholars** (30 total): Alberto Striolo (U. Oklahoma), Jerome Delhommelle (U. South Carolina), Y. Leng (George Washington University), Lukas Vleck (Oak Ridge National Laboratory), Hugh Docherty (Bryan Engineering), Adam Skelton (U. Dayton), Michael Rouha (Czech Academy of Sciences), Junhwan Jeon (current), Guang Feng (current), Stephan Hlushak (current), Ming-Jie Wei (current)

Total Graduate Students Advised: 59 (29 M.S., 30 Ph.D.)

Total Postdoctoral Scholars Advised: 30