

J. David Schall

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Education

- **Ph.D. in Materials Science and Engineering**, North Carolina State University, 2004, *Dissertation*: "Computational Modeling: Nanoindentation and an *Ad Hoc* Molecular Dynamics-Finite Difference Thermostat." (Under the direction of Donald W. Brenner.)
- **M.S. in Materials Science and Engineering**, North Carolina State University, 2000, *Dissertation*: "Computational Study of the Mechanical and Electrical Properties of Carbon Nanotubes with Application to Device Design." (Under the direction of Donald W. Brenner.)
- **B.S. Materials Science and Engineering**, North Carolina State University, 1997, Magna Cum Laud.

Professional Experience

- Assistant Research Professor, Chemistry Department, United States Naval Academy August 2004 to present. *Duties include molecular dynamics simulation of diamond films using reactive empirical bond order potentials and teaching general chemistry courses.*
- Cooperative Learning Experience with prominent researchers in the fields of computational materials science and nanoindentation at Oak Ridge National Laboratory during the summers of 2001 and 2002
- Materials Analyst, IBM-RTP Materials Laboratory, Raleigh North Carolina, 1995-1997. *Duties included materials specification and failure analysis.*
- Research Assistant, Oak Ridge National Laboratory's High Temperature Materials Lab, Thermophysical Properties User Group, 1994. *Duties included implementing the 3 Ω thermal conductivity measurement method and measurement of thermal conductivity in thermal barrier coatings for G.E. Aircraft Engines turbine blades.*

General Research Interests

Prediction of the structure, mechanical, thermal transport and electronic properties of advanced materials using atomistic molecular dynamics simulations and hybrid multiscale modeling approaches. *Recent areas of application include:*

- Friction and tribochemistry of hard coatings
- Structure and mechanical properties of diamond-like carbon films
- Fullerene-based materials and nanocomposites
- Interatomic potential fitting for metallic-covalent systems

A detailed summary of past and present research and as well as copies of selected papers may be found at: <http://www.usna.edu/Users/chemistry/schall/>

Summary of Publication Record

- Total Refereed Publications: 17
- Major Review Articles and Book Chapters: 7
- Number of Citations (as of December 2007): 89

Teaching Experience

- General Chemistry with Naval Applications. (Introductory course: 4 credit hours including 1 hour laboratory credit and weekly recitation sessions)
- Mentoring undergraduate research in Computational Chemistry, 2006
- Mentoring undergraduate research in Computational Materials Science, 2002

Computational Methods Employed

- Reactive empirical bond-order potentials (Brenner, Tersoff, etc.)
- Embedded atom method
- Modified embedded atom method
- Semiempirical tight-binding – electronic structure calculations
- *Ab initio* calculations using Gaussian
- Potential fitting
- Finite difference methods for heat flow, diffusion, etc.

Honors and Awards

- Co-recipient of the Feynman Award for Research in Nanotechnology (theory), 2002
- Co-Principal Investigator: North Carolina Supercomputing Center research grants 1997-2003
- Awarded NSF-SRC travel grant to present at 2002 Trends in Nanotechnology Conference in Santiago de Compostela, Spain.
- SURA-ORNL: Summer Cooperative Research Program in Materials Science grant recipient 2001, 2002
- Co-author, Veridian Medal Paper, 1999