



William F. Polik

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 Professor of Chemistry
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Education:

B.A., Dartmouth College, 1982

Ph.D., University of California, Berkeley, 1988

Areas of expertise: high-resolution laser spectroscopy, highly excited molecular states, computational chemistry, educational software

Grants and awards:

- "Transportable Pulsed Laser System to Enhance Undergraduate Research Programs" 2004-07, \$242,000
- "Acquisition of a Computer Cluster for Research, Research Training, and Teaching", 2005-08, \$380,000
- "Structure and Spectroscopy of Open-Shell and Electronically Excited Species", 2006-11, \$187,000

Key publications and presentations:

- K.E. Hahn and W.F. Polik, "Factors Influencing Success in Physical Chemistry", *J. Chem. Ed.* 81, 567 (2004)
- M.A. Cortez, N.R. Brinkmann, W.F. Polik, P.R. Taylor, Y.J. Bomble, and J.F. Stanton, "Factors Contributing to the Accuracy of Harmonic Force Field Calculations for Water," *J. Chem. Theory and Comp.*, in press (2007)

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Laser Spectroscopy of Highly Excited Vibrational States:

Dispersed fluorescence spectroscopy of molecules in a free jet has produced the most detailed experimental characterization of polyatomic molecular potential energy surfaces ever recorded.



High Accuracy Computation of Molecular Potential Energy Surfaces and Properties:

A cluster computer works in parallel to complete weeklong calculations in hours, allowing rapid testing of chemical theories and accurate prediction of chemical properties.

Web-Based Software for Computational Chemistry:

WebMO is the most widely used web interface to popular computational chemistry programs, such as Gaussian, Gamess, Mopac, Molpro, NWchem, and Qchem.

