

## DAVID A. DIXON

Robert Ramsay Professor of Chemistry, University of Alabama

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### Education

California Institute of Technology, Pasadena, CA, Chemistry, B.S. with honors, June 1971  
Harvard University, Cambridge, MA, Physical Chemistry, March 1976

### Positions Held

Robert Ramsay Chair, Chemistry, U. Alabama, Tuscaloosa, AL, 2004 -present  
Pacific Northwest National Laboratory, Richland WA, Battelle Fellow 2002-2003,  
Associate Dir., Theory, Modeling & Simulation, Environm. Molec. Sci. Lab., 1995-2002  
Member of Research Staff, Chemical Sciences, Central Research and Development Department,  
E.I. du Pont de Nemours and Co., Inc. Wilmington, DE, 1983-1999; Research Fellow, 1992-1995;  
Research Leader, in computational chemistry, 1990-1995.  
Assistant Prof., Chem. Department, U. Minnesota, Minneapolis, MN, 1977-1983.  
Visiting Associate, Chem., California Inst. of Technology, Pasadena, CA, 1977-1977.  
Junior Fellow, Society of Fellows, Harvard University, Cambridge, MA, 1975-1977.

### Selected Awards and Synergistic Activities

1977-1981 Alfred P. Sloan Research Fellowship  
1978-1983 Camille and Henry Dreyfus Teacher-Scholar  
1988-present Editorial Board *International J. High-Performance Computing Applications*  
1989 Leo Hendrik Baekeland Award of the American Chemical Society  
1994 Fellow - American Association for the Advancement of Science  
2002 Fellow of the American Physical Society, Division of Chemical Physics  
2003 American Chemical Society Award for Creative Work in Fluorine Chemistry  
2006 U. of Alabama Computer Based Honors Program, Outstanding Project Director  
2007 20<sup>th</sup> Annual Charles A. Coulson Lecture, University of Georgia

### 5 related Publications (out of ~500, 3 patents, >225 presentations)

- M. T. Nguyen, M. H. Matus, V. E. Jackson, V. T. Ngan, J. R. Rustad, and D. A. Dixon,  
"Mechanism of the Hydration of Carbon Dioxide: Direct Participation of H<sub>2</sub>O versus  
Microsolvation," *J. Phys. Chem. A*, WEB ASAP Sept. 2008;  
S. Li and D. A. Dixon, "Molecular Structures and Energetic of the (TiO<sub>2</sub>)<sub>n</sub> (n = 1-4) Clusters and  
Their Anions," *J. Phys. Chem. A* **112**: 6646 (2008).  
D. A. Dixon, J. S. Francisco, and K. O. Christe, "Bond Dissociation Energies in Second Row  
Compounds," D. J. Grant, M. H. Matus, J. Switzer, *J. Phys. Chem. A* **112**: 3145 (2008).  
S. Li, K. A. Peterson and D. A. Dixon, "Benchmark Calculations on the Adiabatic Ionization  
Energies of the M-NH<sub>3</sub> (M = Na, Al, Ga, In, Cu, Ag) Complexes," *J. Chem. Phys.* **128**:  
#154301 (2008).  
W. J. Shumate, D.L. Mattern, A. Jaiswal, D. A. Dixon, T.R. White, J. Burgess, A. Honciuc, and  
R.M. Metzger, "Spectroscopy and Rectification of Three Donor-Sigma-Acceptor  
Compounds, Consisting of a One-Electron Donor (Pyrene or Ferrocene), a One-Electron  
Acceptor (Perylenebisimide), and a C<sub>19</sub> Swallowtail," *J. Phys. Chem. A* **110**: 11146-11159  
(2006).

### 5 Related publications

- J. L. Gole, E. Veje, R.G. Egeberg, A. Ferreira da Silva, I. Pepe, and D. A. Dixon, "Optical Analysis  
of the Light Emission From Porous Silicon: A Hybrid Polyatom Surface-Coupled  
Fluorophor," *J. Phys. Chem. A* **110**: 2064 (2006).

- K. E. Gutowski and D. A. Dixon, "Predicting the Energy of the Water Exchange Reaction and Free Energy of Solvation for the Uranyl Ion in Aqueous Solution," *J. Phys. Chem.* **A110**: 8840 (2006).
- P. W. Kletnieks, A. J. Liang, R. Craciun, J. O. Ehresmann, D. M. Marcus, V. A. Bhirud, M. M. Klaric, M. J. Hayman, D. R. Guenther, O. P. Bagatchenko, D. A. Dixon, B. C. Gates, and J. F. Haw, "Molecular Heterogeneous Catalysis: A single-site Zeolite-Supported Rhodium Complex for Acetylene Cyclotrimerization," *Chem. Eur. J.* **13**: 7294 (2007).
- K. E. Gutowski and D. A. Dixon, "Ab Initio Prediction of the Gas- and Solution-Phase Acidities of Strong Brønsted Acids: The Calculation of  $pK_a$  Values Less Than -10" *J. Phys. Chem.* **A110**: 12044 (2006).
- K. E. Gutowski, J. D. Holbrey, R. D. Rogers, and D. A. Dixon, "The Prediction of the Formation and Stabilities of Energetic Salts and Ionic Liquids from *Ab Initio* Electronic Structure Calculations," *J. Phys. Chem.* **B109**: 23196 (2005).

**Collaborators (last 48 months):** C. Aardahl (PNNL), A.J. Arduengo (UA), T. Autrey (PNNL), R.T. Baker (LANL), M. Bakker (UA), S. Blackstock (UA), J.A. Boatz, (Edwards AFB), M. Bowman (UA), C. Burda (Case Western U.), P. Burns (Notre Dame U.), A. K. Burrell (LANL), W. H. Casey (U.C.-Davis), C. Cassady (UA), K. O. Christe (U. So. Cal.), W.A. deJong (PNNL), Z. Dohnalek (PNNL), R.G. Egeberg (Niels Bohr Inst.), A. Federov (Ga Tech), A. Ferreira da Silva (U. Federal da Bahia, Brazil), D. Feller (PNNL), A.R. Felmy (PNNL), J.S. Francisco (Purdue U.), B.C. Gates (U.C.-Davis), K.I. Goldberg (U. Wash.), J.L. Gole (Ga Tech), M.S. Gordon, (Iowa St. U.), A. Gupta (UA), M. Gutowski (Herriot-Watt U., Edinburgh), R.J. Harrison (ORNL), J.F. Haw (U. So. Cal.), M.F. Hawthorne (U. Missouri), B.P. Hay (ORNL), D.M. Heinekey (U. Wash.), J.Z. Hu (PNNL), E. Iglesia (U.C.-Berkeley), J. Jones-Oliveira (PNNL), S.M. Kauzlarich (U.C.-Davis), B. Kay (PNNL), L. Kispert (UA), A. Lane (UA), J. Linehan (PNNL), J. Liu (PNNL), D. McDonald (Penn St. U.), T.B. McMahon (U. Waterloo), H.P.A. Mercier (McMaster U.), R. Metzger (UA), J.A. Nichols (ORNL), D. Nikles (UA), J.S. Oliveira (PNNL), S. Pan (UA), C. Peden (PNNL), I. Pepe (U. Federal da Bahia, Brazil), K.A. Peterson (Wash. St. U.), C. Pittman (Miss. State), P.P. Powers (U.C.-Davis), S.M. Prokes (NRL), R.D. Rogers (UA), J.R. Rustad (U.C.-Davis), G.J. Schrobilgen (McMaster U.), K.H. Shaughnessy (UA), L.G. Sneddon (U. Penn.), T.S. Snowden (UA), L. Soderholm (ANL), F.H. Stephens (LANL), T.P. Straatsma, (PNNL), S. Street (UA), G. Szulczewski (UA), M. Tamm (Braunschweig), D.L. Thorn (LANL), W. Tumas (LANL), H. Turner (UA), T. Vaid (UA), L.-S. Wang (Wash. St. U.), Y. Wang (PNNL), W.W. Wilson (Univ. So. Cal.), T.L. Windus (Iowa State U.), M. White (Miss State), S. Woski (UA), C-G. Zhan (U. Kentucky)

**Thesis Supervisors:** Professors D.R. Herschbach and W.N. Lipscomb, Emeritus, Chemistry Department, Harvard University

**Former PhD Students (U. Mn):** Robert A. Eades (IBM Life Sciences, University & Government), Steven C. Richtsmeier (Spectral Sciences, Burlington Ma), Robert Glinski (Professor, Chemistry, Tennessee Tech), David Weil (3M Corporate Technology Center), Mark Ellenberger (Technical Director, Minnesota Revels).

**Former graduate students UA:** Keith Gutowski (PhD, 12/2006, postdoc, Notre Dame)

**Current PhD students (UA):** Raluca Craciun (5<sup>th</sup> yr), Daniel Grant (4<sup>th</sup> year), Virgil Jackson (4<sup>th</sup> year), Tsang-Hsui Wang (3<sup>rd</sup> year), Mingyang Chen (2<sup>nd</sup> year), Jason Dyer (1<sup>st</sup> yr), Amanda Stott (1<sup>st</sup> year), Ted Garner (1<sup>st</sup> yr).

**Postdoctorals (PNNL):** J. Garza Asst. Prof. (U. Auton. Metrop.-Iztapalapa, Mexico), R. Vargas Asst. Prof. (U. Auton. Metrop. Iztapalapa, Mexico), G. Sandrone, Italian Pharmaceutical Company, C.-G. Zhan (Assoc. Prof., School of Pharmacy, U. Kentucky)

**Current Postdoctorals (UA):** Shenggang Li (U. Kentucky), Myrna Hernandez-Matus (Auton. Metrop. U. – Iztapalapa, Mexico), Visiting Prof. M. Nguyen (Leuven)

**Undergraduate students (UA):** Supervised >25 students in Computer Based Honors Program, undergraduate thesis, REU since arriving at UA in 1/2004.