

# H. Bernhard Schlegel

## Education:

University of Waterloo, Waterloo, Ontario, Canada, B.Sc. (Honors Chemistry), 1972  
Queen's U, Kingston, Ont. Canada, Ph.D. (Theor. Organic Chemistry) with S. Wolfe, 1975  
Princeton University, Postdoctoral Fellow with K. Mislow and L.C. Allen, 1976-77  
Carnegie-Mellon University, Postdoctoral Research Associate with J.A. Pople, 1977-78

## Appointments and Professional Experience:

Distinguished Professor, Wayne State U., 2011 – present,  
Prof. 1985 - 2011, Assoc. Prof. 1984 - 1985, Assist. Prof. 1980 - 1984  
Associate Editor, Journal of Chemical Theory and Computation, 2011 -  
Adjunct Professor, University of Utah, 2000 - 2008  
WSU Institute for Scientific Computing, 2000 - 2007  
WSU Institute for Drug Design, 2000 - 2003  
Lecturer, NATO Advanced Study Institutes (Menton, Fr. 7/80; Sant Feliu de Guixols, Sp. 7/88; Altinoluk,  
Turkey, 8/89; Porto Novo, Port. 8/90; Porta Delgada, Azores, 8/92)  
Lecturer, Gaussian Workshops (1991 - present).  
Senior Research Chemist, Merck, Sharp & Dohme Research Labs, Rahway, NJ, 1978 - 1980

## Honors and Awards:

ACS Award for Computers in Chemical and Pharmaceutical Research, 2013  
International Academy of Quantum Molecular Science, 2011 - present  
Fellow of the American Chemical Society, 2011 - present  
Fellow of the Royal Society of Chemistry, 2009 - present  
Fellow of the American Association for the Advancement of Science, 2009 - present  
Wayne State University Outstanding Graduate Mentor Award, 2007  
Wayne State University Distinguished Faculty Award, 2003  
Wayne State University Academy of Scholars, 2001 - present  
WSU College of Science Teaching Award, 2002  
WSU Charles H. Gershenon Distinguished Faculty Fellowship, 2000 - 2002  
Wayne State University Career Development Chair, 1985-86  
Camille and Henry Dreyfus Teacher-Scholar, 1984-89  
Alfred P. Sloan Fellowship, 1981-83  
National Research Council of Canada NATO Postdoctoral Fellowship, 1976-78  
National Research Council of Canada 1967 Centennial Scholarship, 1972-75  
Ford Motor Company Scholarship, 1969-72

Former and Present Students Carlos Sosa (PhD, 1986), Xiaoxia Ma (MS, 1988), Edgar Ignacio (PhD, 1990), Carlos Gonzalez (PhD, 1990), Gary Fox (PhD, 1992), Cynthia Darling (PhD, 1993), Wei Chen (PhD, 1994), Anwar Baboul (PhD, 1997), Felix Martinez (PhD, 1997 joint with M. Newcomb), Philippe Ayala (PhD, 1997), Joanne Wittbrodt (PhD, 1999), Mathew Halls (PhD, 2001), Jason Cross (PhD, 2002), Xiaosong Li (PhD 2003), John Knox (PhD 2005), Smriti Anand (PhD 2005), Hrant Hratchian (PhD 2005), Jie Li (PhD 2006), Stanley Smith (PhD 2006), Michael Cato (MSc 2008), Barbara Munk (PhD 2009), Jia Zhou (PhD 2011), Jason Sonk (PhD 2012); Brian Psciuk (PhD 2013); Adam Birkholtz (PhD 2015); Xuetao Shi; Bishnu Thapa; Yi-Jung Tu; Sebastien Hebert, Paul Hoerner

Post-docs G. Tonachini (1983-5), J. McDouall (1987-9), J. Andrés (1989-91), M-D Su (1992-3); C. Y. Peng (1992-4), Ö. Farkas (1996-8), J. Wittbrodt (1999-2000), J. Millam (1997-2001), J. Sonnenberg (2005-2009), Peng Tao (2007-2010), Richard Lord (2010-2012), Suk-yung Lee (2010-2012), Pascal Krause (2012-2015), Shivnath Mazumder (20013 - 2016), Qing Liao (2015 - )

Collaborators G. Voth (U. Chicago), C. Burrows (U. Utah), S. Mobashery and J. Fisher (Notre Dame), R.J. Levis (Temple U.), S. Shaik (Hebrew U.), G. Scuseria (Rice U.), Ö. Farkas (Eötvös U., Budapest), J. Montgomery and T. Goodson (U. Mich.), C. H. Winter, C. Verani, J. F. Endicott, W. Li, J. Cha and J. Kodanko (Chemistry, Wayne State U.), D. Gatti and B. F. P. Edwards (Med. School, Wayne State U.), P.G. Wang (Georgia State U.), M.A. Robb (Imperial College, London), M. J. Frisch (Gaussian), H. P. Hratchian (UC-Merced), M. Caricato (U. Kansas), T. Vreven (Med. School, U. Mass.)