

Institute Lecture

Density Cumulant Theory

Prof. Henry F. Schaefer, III



Graham Perdue Professor of Chemistry, Director of the Center for Computational Quantum Chemistry, University of Georgia

22nd March 2017, Time: 6:30 PM, Venue: Outreach Auditorium

Abstract

For the past several years we have been developing a new theoretical method, regrettably labeled Density Cumulant Functional Theory by Werner Kutzelnigg. Density Cumulant Theory (DCT), our preferred name, has virtually nothing to do with Density Functional Theory, now becoming (in practice) primarily a highly parameterized semi-empirical method. The new theory DCT will be reviewed, with some of the most recent methodological advances exploiting symmetry, parallelization, and density fitting. Applications will be reported.

About the speaker

Professor Henry F. Schaefer III was born in Grand Rapids, Michigan. He attended public schools in Syracuse (New York), Menlo Park (California), and Grand Rapids (Michigan), graduating from East Grand Rapids High School. He received his B.S. degree in chemical physics from the Massachusetts Institute of Technology and Ph.D. degree in chemical physics from Stanford University. For 18 years he served as a professor of chemistry at the University of California, Berkeley. During the 1979-1980 academic year he was also Wilfred T. Doherty Professor of Chemistry and inaugural Director of the Institute for Theoretical Chemistry at the University of Texas, Austin. Since 1987 Dr. Schaefer has been Graham Perdue Professor of Chemistry and Director of the Center for Computational Quantum Chemistry at the University of Georgia. He is the author of more than 1500 scientific publications. Critical to Professor Schaefer's scientific success has been a brilliant array of students and coworkers; including 68 undergraduate researchers who have published papers with him, 111 successful Ph.D. students, 51 postdoctoral researchers, and 80 visiting professors who have spent substantial time in the Schaefer group. He is the recipient of 31 honorary degrees. He was the longest serving Editor-in-Chief of the journal *Molecular Physics* (1995-2005). He is currently Associate Editor for the journal *Physical Chemistry Chemical Physics*. He was also the longest (1996-2005) serving President of the World Association of Theoretical and Computational Chemists. On March 29, 2012 Professor Schaefer received the \$20K SURA Distinguished Scientist Award, given to the most outstanding scientist in any field. In October 2012 "The Best Schools" identified him as one of seven chemists deserving of a *Nobel Prize*. Most recently he received the American Chemical Society Peter Debye Award.

Tea at 6:15 PM

All interested are welcome.

S. Ganesh
Dean of Research and Development, IIT Kanpur