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The Mysteries of Chirality, Solvation, and Optical Activity

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ABSTRACT

The optical properties of chiral molecules are among the most challenging to predict and simulate — even for state-of-the-art quantum chemical methods — because of their delicate dependence on a variety of intrinsic and extrinsic factors, including electron correlation, basis set, vibrational/temperature effects, etc. In numerous studies over the last decade, we have demonstrated the importance of advanced quantum chemical methods such as coupled cluster response theory for the prediction of an array of gas-phase chiroptical properties such as optical rotation angles, circular dichroism rotatory strengths, Raman optical activity scattering intensity differences, and more. The primary disadvantage of such methods, however, is their high-degree polynomial scaling, which limits significantly the size of system to which they may be applied. Furthermore, solvation makes the task even more difficult, not only dramatically expanding the complexity of the simulation, but sometimes altering even the sign of the chiral response. It is thus essential that we reduce the computational demands of the more accurate and reliable quantum chemical methods. This lecture will explore the many ways in which we are pursuing both more efficient theoretical models of optical activity, but means for extracting deeper understanding from them.

BIO:

T. Daniel Crawford was raised in Morgan County, Alabama, on his parents' cattle farm in the Appalachian foothills. He attended public school in the small town of Arab, Alabama, where he was fortunate to have many talented teachers who sparked his interests in science and mathematics. He received his bachelor's degree in chemistry and mathematics in 1992 from Duke University, where he also engaged in undergraduate research with Prof. Weitao Yang. He held a National Science and Engineering Graduate Fellowship from the U.S. Department of Defense and the Fritz London Graduate Fellowship under Prof. Henry F. Schaefer at the University of Georgia's Center for Computational Quantum Chemistry, where he completed his Ph.D. in 1996. From 1996 to 2000, he held joint postdoctoral positions with Prof. Schaefer at Georgia and with Prof. John Stanton at the University of Texas. In May of 2000, Dr. Crawford was appointed assistant professor of chemistry at Virginia Tech, in Blacksburg, Virginia, followed by promotion to associate professor in 2005 and then to full professor in 2009.