



CHEMISTRY & BIOCHEMISTRY COLLOQUIUM: First Principles Simulations of the Optical Rotation in Oriented Systems

Marco Caricato

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Date:

12/2/2022

Time:

1:30 PM - 2:50 PM

Location:

COB 267

About The Speaker:

Marco Caricato earned his M.S. in Chemistry at the Università di Pisa (Italy) in 2003 and his Ph.D. in Chemistry at the Scuola Normale Superiore (Italy) in 2006 under the supervision of Jacopo Tomasi. From 2006 to 2010, he worked as a postdoctoral researcher with Ken Wiberg at Yale University and from 2010 to 2014 as a research scientist at Gaussian, Inc., before becoming a professor at the University of Kansas in 2014. His research interests involve the development and application of quantum mechanical methods to condensed phase systems for the investigation of reactivity, catalysis, and light-matter interactions.

Abstract:

This contribution presents simulations of the optical rotation of chiral crystals using periodic density functional theory methods. The full Buckingham-Dunn tensor is computed using a periodic formalism for the electric dipole, magnetic dipole, and electric quadrupole integrals. The approach is used on a variety of test systems to investigate the effect of the choice of approximate functional, basis set, and gauge for the electric dipole operator. The effect of intermolecular interactions is also investigated and compared to the intrinsic optical rotation of chiral molecular units.