UCMERCED
UNIVERSITY OF CALIFORNIA
School of Natural Sciences

CHEMISTRY SEMINAR 291

Exploring the Electronic and Vibrational Structure of Carbon Dioxide

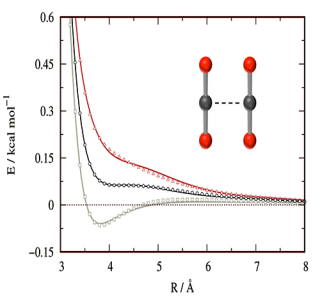
Olaseni Sode
Department of Chemistry and Biochemistry
California State University, Los Angeles

Date: 2/1/19
Time: 1:30 PM
Location: COB1 267

For more information contact:
Michelle Leslie
jmleslie@ucmerced.edu

ABSTRACT

A "first principles" many-body carbon dioxide potential energy function (mbCO2) is developed for CO2 gas and condensed phase systems. The mbCO2 potential was originally constructed as a dimer potential function with flexible-monomers calculated at the CCSD(T)-F12b/aug-cc-pVTZ level of theory. Recently, we have included three-body contributions, expressed as the sum of permutationally invariant polynomials and the Axilrod-Teller-Muto three-body function, and derived from a fit to over 15,000 CO2 trimer configurations calculated at the CCSD(T)-F12a/aug-cc-pVDZ level. With the updated many-body potential, we revisit the optimization of CO2 clusters as well as the energetic ordering of trimers. Anharmonic frequencies are determined using correlated vibrational structure methods and compared to experimental values with special attention directed at the intermolecular modes of vibration.



BIO:

Olaseni Sode attended Morehouse College and received a B.S. in Chemistry and a B.A. in French in 2007. He began graduate school at the University of Florida (UF) where he worked under the supervision of Professor So Hirata. His research here focused on studying molecular crystals (e.g. hydrogen fluoride, solid water, and solid carbon dioxide) using ab initio electronic and vibrational structure methods. After completing his candidacy at UF, he continued his graduate studies at the University of Illinois at Urbana-Champaign (UIUC) accompanying his graduate advisor. He earned his Ph.D. from UIUC in 2012. From 2012 to 2015, he conducted postdoctoral research at The University of Chicago under the advisement of Professor Gregory A. Voth. Here, he studied the physical processes in multiscale chemical systems using coarse-grain modeling, enhanced sampling techniques and multistate reactive molecular dynamics. In 2015, he began his independent career as an assistant professor at The University of Tampa in the Department of Chemistry, Biochemistry and Physics. Professor Sode's research projects have been funded by the National Science Foundation and the American Chemical Society Petroleum Research Fund. Recently, he was awarded the Florida Education Fund's Junior Faculty Development Fellowship. His long-term research goals focus on the development of model potentials exploiting fragmentation quantum chemistry methods to address condensed phase molecular systems at the highest levels of electronic structure theory. In the fall of 2018, Olaseni Sode moved to California State University, Los Angeles.