Exploring the electronic and vibrational structure of CO_2 clusters

Olaseni Sode

The University of Tampa, Department of Chemistry, Biochemistry and Physics, Tampa, FL, 33606.

A "first principles" many-body carbon dioxide potential energy function (*mb*CO2) is developed for CO_2 gas and condensed phase systems. The *mb*CO2 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 CO_2 trimer configurations calculated at the CCSD(T)-F12a/aug-cc-pVDZ level. With the updated many-body potential, we revisit the optimization of CO_2 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.