ab initio Calculations of Optical Absorption in Planar Boron Wheels

Ravindra Shinde[1] and Alok Shukla[1]

[1] *Department of Physics, Indian Institute of Technology Bombay, Mumbai,*

The linear optical absorption spectra of planar boron clusters (B_7 , B_8 and B_9) in wheel shapes are calculated using a systematic all-electron correlated calculation approach. The geometries of these clusters were optimized at the coupled-cluster singles doubles (CCSD) level of theory. With these optimized geometries, excited states were computed using the equation-of-motion coupled cluster singles doubles (EOM-CCSD) approach. This is a popular approach to include the electron correlation in large molecules and clusters at a sophisticated level. Also bench-marking this high-level calculations were done with respect to time-dependent density functional (TDDFT) calculations and configuration interaction singles (CIS) calculations. The nature of optical excitation involved are found to be of collective, plasmonic type, by noticing the contribution of configurations to many body wavefunctions.