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Electronic Structure and Potential Fitting Methods Suitable For Multistate Reactive Surfaces

RICHARD DAWES, Missouri University of Science and Technology

Part of this talk describes the development of a PES generator (software code) which uses parallel processing on High-Performance Computing (HPC) clusters to construct PESs automatically. Thousands of *ab initio* data are computed at geometries chosen by the algorithm and fit to a functional form. The electronic structure of molecules is difficult to describe continuously across global reactive PESs since it changes qualitatively as bonds are formed and broken along reaction coordinates. I will discuss a high-level *ab initio* method (GDW-SA-CASSCF/MRCI) designed to allow the electronic wavefunction to smoothly evolve across the PES and provide an accurate and balanced description of the various regions. These methods are combined to study a number of small gas-phased molecules from the areas of atmospheric, combustion and interstellar chemistry including a large variational calculation of all the bound vibrational states of ozone and the photodissociation dynamics of the simplest Criegee intermediate (CH_2OO).