AUTOMATIC COMPUTATION OF GLOBAL INTERMOLECULAR POTENTIAL ENERGY SURFACES FOR QUANTUM DYNAMICAL SIMULATIONS

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We aim at simulating full quantum mechanically the processes of adsorption and photoreactivity of NO_2 adsorbed on soot particles modeled as large Polycyclic Aromatic Hydrocarbons in atmospheric conditions. A detailed description of these processes is necessary to understand the differential day-nighttime behavior of the production of HONO (Guan *et al*). In particular, the specific mechanism of the soot-mediated interconversion between NO_2 and HONO is to date not fully understood. The first stage in this study consisted in the determination of all transition states and minima of the NO_2-Pyrene system. To this end, we have used the van der Waals Transition State Search Using Chemical Dynamics (vdW-TSSCDS) method (Kopec *et al*). Starting from a single input geometry, vdW-TSSCDS permits the characterization of the topography of a intermolecular Potential Energy Surface (PES) in a fully automated fashion. This topographical information is used to obtain a global description of the interaction potential, necessary for the dynamical elucidation of spectroscopic properties. For this, we have developed the Specific Reaction Parameter Multigrid POTFIT (SRP-MGPF) algorithm and associated software (Panadés *et al*). This method computes chemically accurate PESs through reparametrization of semiempirical methods which are subsequently tensor decomposed using MGPF. This software has been interfaced with the Heidelberg version of the Multiconfiguration Time-Dependent Hartree (MCTDH) package [8].

References

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