Networked computing for ab-initio modeling the chemical storage of renewable energy

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After the reactive scattering probabilities obtained for the OH + H_2 system using the Quantum-Classical method, the research has continued by investigating the non reactive scattering processes. The conditions needed fot the inelastic analysis of the non reactive scattering processes, have evidenced the inability of the until then used PES in order to describe correctly the intermolecular long range potential. A Potential energy tail based on the Improved Lennard Jones potential and the electrostatic quadrupole-dipole interacion have been developed and added to the until then used Potential energy surface. Reactive and inelastic rate constants have then been calculated by simulating the scattering processes with the new PES. The comparison of the results obtained with the experimental ones available in literature showed an excellent agreement and a clear increase in accuracy of the obtained results. Its success encouraged the development of a more general approach, a Potential Energy fitting method able to intrinsically predict the long range behaviour. The Bond Order expansion fitting method has thus been started to develop in order to reach that goal.

Ru nanoparticles acting as Sabatier catalyst have been started to study by means of DFTB method. Validation of the parameters used in the calculations have been carried out by comparing DFTB results with the ones obtained from DFT method for small nanoparticles. The excellent agreement will allow to perform calculations on bigger nanoparticles, performing global optimization using Parallel Tempering method and run the dynamics to see the Role of the Ru nanoparticles acting as Sabatier reaction catalysts. After the failure of the kinetic study using data from literature, calculations of the energy barriers of the steps composing an extended mechanism for the Sabatier reaction have also been performed.