Developments in quantum parametric methods using parameterization techniques and new functionals and applications

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In this work a new parameterization scheme is presented based on properties of parametric functionals (PF) [1] and in particular employing the simplified generalized simulated annealing (SGSA) [2] method. The parameter sensibility study was considered in order to carry out a more efficient search. Other parameterization techniques were employed [3, 4], such as evolutionary algorithms, SIMPLEX, and gradient method.

All parameterization modules were parallelized together with surface process modules implemented to analyze reactivity of materials employed as catalysts. The last modules were adapted to nano-particle calculations and their interaction with adsorbates. Programs based on parameters allow the evaluation of multiple properties at low computational cost. A modular architecture is used to model nanoparticle properties, ducking, adsorption screening , reaction path, transition state, diffusion, desorption, and effects of dopants.

Applications to interstellar reactions are shown as example of molecular fragments on a model graphite grain using a polyaromatic hydrocarbon (PAH), such as coronene. An analysis of different processes is carried out for adsorption sites, coverage, diffusion and adsorption barriers, and different adsorbed intermediates. The formation of diatomic (H-H, C-H, N-H, and OH), triatomic (CH_2, NH_2, and OH_2) as well as polyatomic molecules (CH_4, NH_3, CH_3OH, COOH, etc) are reported.

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Referencias:

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