Quest for shape, energetics and reaction dynamics of molecules

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The most notable approximation in Physics and Chemistry is due to Born and Oppenheimer whereby the electronic and nuclear motions are disentangled and treated separately. Here briefly revisited, the BO approximation is at the heart of the molecular shape concept as well as the study of the energetics and dynamics of chemical reactions. Regarding the molecular shape, we show how it can be explained without calculations on the molecule itself, thus avoiding any criticism of tautology. In an attempt to cost-effectiveness, an extrapolation approach for accurate energies and other molecular properties is discussed. Global ab initio-based potentials are then reported from the double many-body expansion (DMBE) and combined-hyperbolic-inverse-power-representation (CHIPR) formalisms. Due to overwhelming difficulty in calculating potentials for large molecules, the predictive capability of DMBE theory when truncated at the first few-body terms is examined. Finally, recent work in both quasi-classical and quantum reaction dynamics is briefly surveyed, and an attempt to a cost-effective extrapolation approach suggested. Prospective remarks end the talk.