CELEBRATION OF THE 150TH ANNIVERSARY OF THE PERIODIC TABLE
ACADEMIA DAS CIÊNCIAS DE LISBOA,
OCT. 3RD, 10TH, 17TH AND NOV. 21ST / 3 PM

Cost-effective Dual-strategy For Molecular Reaction Dynamics and the Challenging Carbon Clusters

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The talk begins by addressing the Born-Oppenheimer approximation.[1] Two other issues then follow. Firstly, a cost-effective double-strategy for reaction dynamics employing physics-based extrapolation techniques. After surveying recent work on the energetics,[2-4] a recent proposal of optimal basis sets for the direct extrapolation of the potential energy surface is addressed. Non-augmented and diffusely-augmented double-zeta and triple-zeta basis sets of the correlation consistent type are suggested, which are shown to outperform by three- to fivefold the energetics from traditional ansatzes of similar flexibility.[5] Quantum reaction dynamics is next discussed, a topic also demanding huge computational resources.[6,7] Utilizing the correspondence principle as asymptotic theory, extrapolation now resorts on the fact that the laws of quantum theory merge into the ones of classical physics at high energies. With quasiclassical trajectories affordable for most systems, they are then suggested as vehicle for extrapolating quantum zero-total-angular-momentum (J=0) calculations to any J value, thus allowing kinetics studies.[7] Of course, the above dual-strategy cannot yet be claimed as general due to the meager number of applications thus far, particularly to nonadiabatic processes. To illustrate this fact, we finally address recent work on elemental carbon clusters. It is shown that even for small numbers of C atoms, the involved potential energy surfaces can embed intricate topological features with dynamics implications.[8-10] Closing remarks and prospects for future work end the talk.

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