Molecular reaction dynamics. Quasi-classical trajectories and beyond.

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We will discuss how using quasi-classical trajectories, specifically tailored for systems in the gas phase, it is possible to describe and understand reactivity of relatively complex molecules. In particular, it was possible to develop theoretical mass spectrometry [1], with applications from small organic molecules [2] to large peptides [3]. More recently, it was extended to ion-molecule collisions to understand possible reactions in astrophysical conditions [4].
Finally, we will discuss new possible developments to go beyond the quasi-classical trajectories approach and directly include nuclear quantum effects in equations of motions. In particular, this will be useful to consider zero-point energy and tunneling in simulations.

References:
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