Semiclassical vibrational spectroscopy from small molecules to solvated biomolecules

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The hallmark of semiclassical dynamics is the ability to get quantum effects starting from classical trajectories.[1] Therefore, the main challenge semiclassical methods have to face is to demonstrate their accuracy and possibility to be applied even to large and complex systems.[2]
I will show that semiclassical dynamics can be straightforwardly interfaced to different descriptions of the potential energy surface (PES), ranging from *ab initio* PESs[3-5] to force fields[6,7] and QM/MM schemes. This allows one to apply semiclassical spectroscopy to the calculation of the quantum vibrational features of very different systems, including not only small molecules characterized by elusive Fermi resonances, like ethanol, or hard-to-assign experimental spectra, like proline, but also large systems like solvated biomolecules. Finally, ongoing efforts to reproduce also the intensity of absorption in the framework of semiclassical dynamics will be illustrated.[8]

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