How many water molecules are needed to solvate one?

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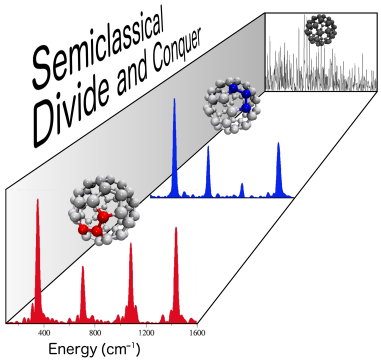
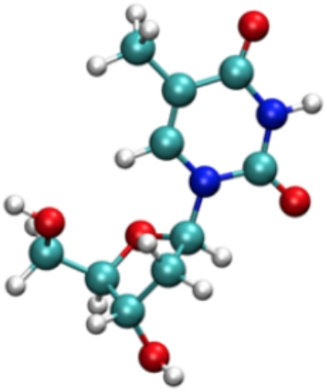
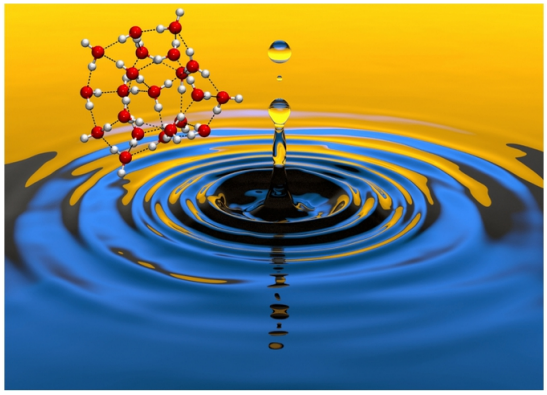
Theoretical vibrational spectroscopy provides a practical way to study both isolated (gas-phase) and solvated systems. When dealing with sizeable molecular systems, the main challenge is represented by the large number of degrees of freedom to be considered. Furthermore, an accurate spectroscopical investigation requires a quantum mechanical treatment, which makes the task even harder to achieve. This key issue involves both the description of the potential energy surface and the molecular dynamics.

Semiclassical dynamics allows one to calculate accurate vibrational spectra with inclusion of quantum effects like zero-point energies, overtones, and quantum resonances starting from short-time classical molecular dynamics runs.[1] In this talk I will briefly introduce the divide-and-conquer semiclassical initial value representation technique (DC SCIVR),[2] and then show a batch of applications involving biomolecules and water-based supramolecular systems.

I will start by demonstrating the spectroscopic accuracy of the technique on isolated (gas-phase) biomolecules (glycine and thymidine).[3-7] Then, I will describe an investigation of water clusters aimed at revealing how many water molecules are needed to have the central monomer featuring the spectroscopic properties of bulk water.[8] Finally, some preliminary results of a study of solvated thymidine will be presented.







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