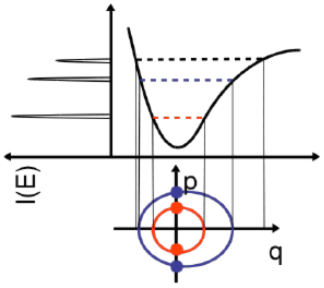
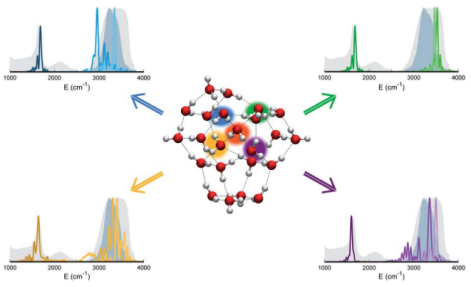
Semiclassical spectroscopy of water clusters using high-level ab initio potentials

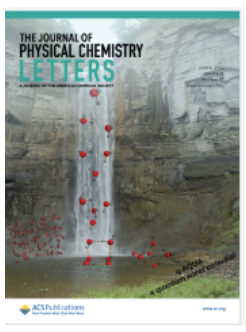
Riccardo Conte, Università degli Studi di Milano, Italy



Semiclassical dynamics as a viable route for vibrational spectroscopy of complex systems



How many water molecules are need to (spectroscopically) solvate one? A semiclassical study of water clusters.



q-AQUA: A new ab initio potential energy surface for water which includes 4-body interactions.