The study of small/medium size molecules inside nanoscale cavities of diverse host material, e.g., clathrates hydrates, cryogenic fluids (or superfluids),fullerenes, carbon nanotubes and zeolites, has received a great deal of attention over the past years due to their broad application domain (condensed matter physics, nanomaterial sciences, geoscience, quantum chemistry, astrophysical and planetary sciences, biophysics, ...). However the description of such systems is often far from complete. Indeed, in such nanoscale confinement, the motion of the encapsulated molecule is far from harmonic and is characterised by large amplitude motions. The translational center-of-mass motions of the caged molecules are quantized and strongly coupled to the molecular rotations, which are quantized too, and also coupled to the internal vibrational motion of the guest molecule.

I will present a review on our recent progress in the development of efficient/accurate computational methods for the rigorous quantum treatment of the intricate coupled translation-rotation dynamics of the molecular hydrogen in water clathrates. In particular, I will emphasize that our methodology enables us to assess the impact of the condensed-phase environment on the vibrational frequency shift of the confined molecule, and at the same time to probe the quality of intermolecular potentials.