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# Coupled translation-rotation bound states of molecular hydrogen in clathrate hydrates from first principles

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## Résumé

The study of small/medium size molecules inside nanoscale cavities of diverse host material, e.g., clathrate 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 translational center-of-mass motions of the caged molecules are quantized and strongly coupled to the molecular rotations, which are quantized too. To interpret experimental data, theoretical tools are useful but we need to go beyond the simple harmonic approximation as the guest molecule presents very large amplitude motions (translation and rotation) and its interaction with the nanoscale cavity can be far from harmonic. A rigorous quantum treatment of the intricate coupled translation-rotation (TR) dynamics of the caged diatomic molecules is far from a routine task.

In this contribution, I will present recent methodological development based on the concept of Smolyak sparse grid technic for the rigorous quantum treatment of the intricate coupled translation-rotation (TR) dynamics of the molecular hydrogen in water clathrates.

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