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Quantum Dynamics with a Smolyak scheme. Applications to clathrate hydrates.

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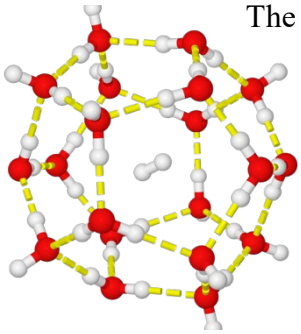
The use of Smolyak scheme in quantum dynamics is an approach that pushes the limits of the current calculations based on a multidimensional basis set and grid. More precisely, the Smolyak scheme[a-c] can be viewed as an approach involving a selection of basis functions and a sparse grid adapted to that basis set. The parameter, L, controls the selection and thus the size of the basis set and grid. With this scheme, the numerical complexity grows as a polynomial of degree L with respect to the number of degrees of freedom d. Systems with up to 12 degrees of freedom can be studied,[d-f] although larger systems (d=21) are possible if few states are needed.[g] This limit can be pushed away using a system-bath separation, and in our Smolyak scheme.[h]



The spectroscopy studies (neutron, Raman …) of encapsulated molecules in cages such as clathrates hydrates (see figure on the left), fullerenes, enable precise characterization of these systems.[i-l] In particular, vibrational shifts and/or translation/rotation motions of the encapsulated molecule provide information about the interactions between the encapsulated molecule and the cage. Results for H_2 or CO encapsulated in rigid or flexible cages will show the efficiency of this sparse grid technique.[m,h]

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