

SEMINAR ANNOUNCEMENT

TUESDAY, 19.04.2016

16:00 h NC 2/99

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Translational/Rotational Dynamics of Confined Species

We describe computational approaches to the elucidation of the quantal translational/rotational dynamics of entrapped molecules and molecular clusters. Our particular focus is on fullerene entrapped species, such as $\text{H}_2\text{O}@C_{60}$ and $\text{H}_2\text{O}@C_{70}$ and on $(\text{H}_2)_N$ clusters entrapped in clathrate hydrate cages. For the latter systems we discuss nuclear-orbital/configuration-interaction methods applied to the dynamics of $(\text{H}_2)_4$ entrapped in the large cage of type- II clathrate hydrate. We also discuss an approach in which the correlated translation motion of the two H_2 moieties in clathrate-entrapped $(\text{H}_2)_2$ is solved for first, the results of which are then used to build up an translation/rotational basis for the solution of the full dynamics of the entrapped $(\text{H}_2)_2$ cluster.

Guests are very welcome!