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Grid empowered molecular simulators of crossed beam signals

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Overview

In the last years, several theoretical and experimental efforts have been spent in the field of quantum reactive scattering and this has fostered the development of molecular simulators [1]. Our group is working at extending GEMS (Grid Empowered Molecular Simulator), to simulate the experimental signal of Crossed Molecular Beams (CMB) experiments. In this communication we report on the implementation of a prototype version of the GEMS block generating the virtual intensity of the product beam of a CMB reactive scattering experiment [2] out of the integration of a large number of quasi-classical trajectories for a three atom reaction.

Impact

The main impact of this work is to be recognized in the possibility of simulating a chemical reaction from the first principles and comparing calculated results directly with those of the related CMB experiment. This affects both the theoretical and experimental sides of dynamical studies. In fact, thanks to this approach the feasibility of a CMB experiment could be predicted a priori by simulating cross sections and possible product distributions. At the same time, on the theoretical side the validity of a proposed potential energy surface could be characterized to a very fine detail if an access to Grid platforms can be obtained. Moreover, the development of the chemical simulator on a Grid environment is also important from a computational science point of view because it prompts the production of specific innovative technological solutions.

Description of the work

GEMS is made of different blocks each of which is devoted to a particular task. In particular, the skeleton of the simulator (the production of ab initio electronic energy values, the fit of these values to work out a potential energy surface and the block devoted to dynamics calculations) has already been designed and implemented whereas the block devoted to the assemblage of the virtual experimental observables is still in the test phase. For this reason, as already mentioned our efforts have been spent in implementing of the last block of the simulator. As a matter of fact, we have designed and implemented on the Grid a Fortran code (called gmtsigma.f) best fitting the measurements of the intensity of the CMB experiments taken as a function of the angle and the velocity of the scattered products (expressed in the laboratory frame) starting out of the related computed dynamical quantities in the Center of Mass (CM) frame (angular distribution, $T(\theta)$, and translational energy distribution, P(E)).

As a study case we have chosen the Cl + H2 system. To this end, an accurate ab initio Potential Energy Surface [3] (PES) has been incorporated inside the quasi-classical trajectory program (VENUS96.F [4]). In order to simulate the observables of the experiment, we have implemented inside the VENUS program the calculation of the fixed angle velocity distribution of the products in the laboratory frame out of the theoretical CM angular and translational energy distributions.

Production runs of the simulator were performed for the system proposed for the study case. To this end, the modified version of VENUS implemented on the GRID was run for 400000 trajectories at different values of the rotational quantum number j. Finally, the comparison between calculated and experimental observables has been carried out.

Conclusions

The design and the implementation of the last segment of the GEMS simulator has been carried out. This means that the simulator is now ready to be used as a powerful instrument in quantum reaction dynamics. We are still in the test phase with respect to the Observables block of the simulator in order to extend the workflow to four atom reactions.
References

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