Modelling the potential energy surfaces and their couplings for nonadiabatic systems.

Scientific report

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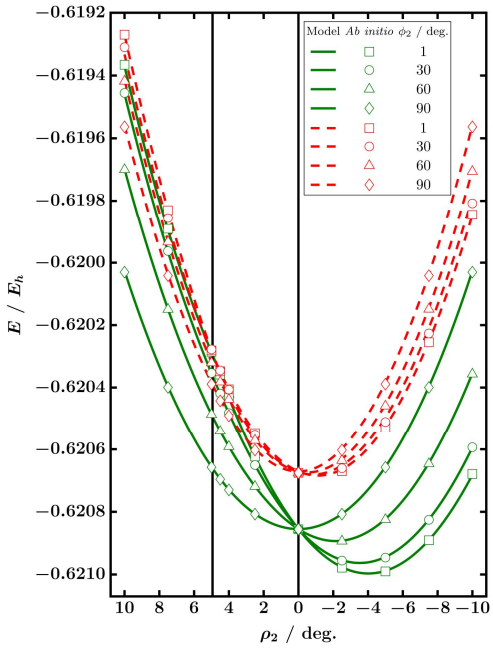

Figure 1. Adiabatic electronic energies for the components of the $X^2\Pi_u$ electronic state of $C_2H_2^+$ as a function of one bending coordinate. [1]

The aim of this project is development of methods for obtaining potential energy surfaces (PES) of small molecule and their couplings that may be used to modeling the dynamics of chemical systems of interest for the Astrochemistry.

During the visit, we discussed the many-body expansion theory (MBE)[2] and the possibility of applying Combined Hyperbolic Inverse Power Representation (CHIRP)[3] of MBE potential energy for systems with more than three atoms. CHIPR approach can offer an accurate scheme to fit a smooth function of the many-body expansion type to a multidimensional large data set using an optimized basis. Although its the applications cover only up to triatomic systems so far, these provide challenging enough tests to warrant promise on its use for larger polyatomics. The plan is investigation of $C_2H_2^+$ ion's PES employing this method, and we performed preliminary quantum mechanical calculations.

[1] M. Perić, S. Jerosimić, M. Mitić, M. Milovanović, R. Ranković, *J. Chem. Phys.* **2015**, 142, 174306.
[2] V.C. Mota, A.J.C. Varandas, *J. Phys. Chem. A* **2008**, 112, 3768.
[3] A.J.C. Varandas, *J. Chem. Phys.* **2013**, 138, 54120.

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