VISTA Seminar

Seminar 72

June 26, 2024

10:00 am – 11:30 am EDT / 3:00 – 4:30 pm BST London / 4:00 pm – 5:30 pm CEST Paris / 10 pm – 11:30 pm CST Beijing

TOC:

Constructing PIP potential energy surfaces for semiclassical vibrational spectroscopy calculations

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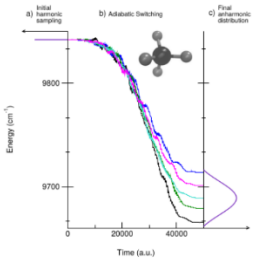

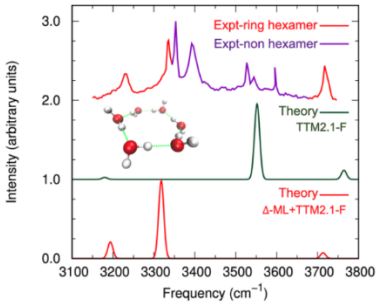

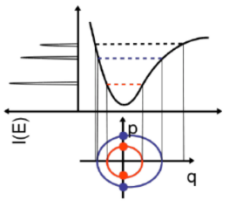

I will start by introducing the technique of permutationally invariant polynomials (PIP) for building high-level, accurate, and fast-to-compute potential energy surfaces (PESs). The PIP technique provides precise fits up to high energies and fast gradient calculation. Furthermore, it is suitable for application of the Δ-machine learning technique to take the PES to a higher level of electronic structure theory. Then, I will briefly describe semiclassical vibrational spectroscopy and show some calculations performed on PIP PESs, pointing out the importance of fitting the PES at high energies and the need for an accurate description of the potential. Finally, I will conclude by introducing a new semiclassical approach to calculate IR spectra based on the time average technique.

How to Estimate the Number of Bonds in Diatomic Molecules from Excited State Potential Energy Curves: A Theoretical Treatise

Ishita Bhattacharjee, Debashree Ghosh and Ankan Paul

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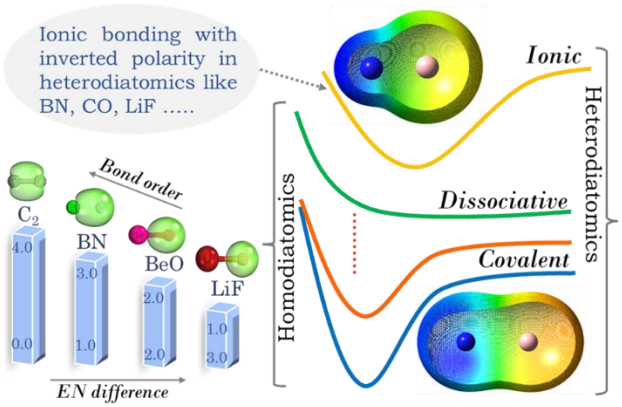

The fundamental concept of chemical bonding is firmly rooted on the studies based on diatomic species. Incidentally, the number of bonds in the ground state of diatomic species C_2 had become a topic of discussion with disagreements preceding over agreements. Although the Kohn-Sham orbitals of ground state of C2 predicts a bond order of 2.0, various contrasting views had been expressed from schools of VB and MO theory.[1-3] Our investigations are focused on seeking a definitive answer to this question by investigating the excited potential energy curves of C_2 and related 2nd period diatomic species. In this project, through the examination of high spin excited state surfaces along with the nature of the dominant Configuration State Functions we would try to establish that one can infer on the number of bonds present in the ground state of a diatomic molecule.[4] Additionally, we would shed light on the strengths and weaknesses of such an approach for counting bonds.

References

1. S. Shaik, D. Danovich, W. Wu, P. Su, H.S. Rzepa and P.C. Hiberty, Nat. Chem. 2012, 4(3), 195.
2. D. Danovich, S. Shaik, H.S. Rzepa and R. Hoffmann, Angew. Chem. Int. Ed. 2013, 52(3), 5926.
3. G. Frenking and M. Hermann, Angew. Chem. Int. Ed. 2013, 52, 5922.
4. I. Bhattacharjee, D. Ghosh and A. Paul, Chem. Sci. 2020, 11, 7009.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 72
Time: Jun 26, 2024 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting
https://buffalo.zoom.us/j/95967485605?pwd=lf3eIdOLbPvLIOmDVa7LHXRlfDoyab.1

Meeting ID: 959 6748 5605
Passcode: 164690