Theoretical Quantum Physics

Group Seminar

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Online (Zoom)

Dissecting Molecular Interactions Using Concepts of Quantum Information Theory

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Abstract

Orbital entanglement and correlation represent a useful and intuitive tool to interpret complex electronic wave functions and facilitate a qualitative understanding of the electronic structure and how it changes in chemical processes[1]. In contrast to conventional interpretive tools exploited in computational chemistry, orbital entanglement and correlation represent a conceptually different approach that can provide much sought-after insights in electronic structure calculations and chemical processes: they can be used to dissect electron correlation effects[2], bond formation processes[3], and changes in the electronic wave function to, for instance, identify transition states. Furthermore, these tools can be used to design optimal active spaces in multi-reference calculations[1,4]. We will start with some proof-of-principle examples such as the dissociation of main-group compounds and the formation of a chemical bond along some reaction pathway[5], and move on to more challenging examples containing heavy-element species.

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[2] K. Boguslawski, P. Tecmer, O. Legeza and M. Reiher, *J. Phys. Chem. Lett.*, 2012, 3, 3129–3135.
[3] K. Boguslawski, P. Tecmer, G. Barcza, O. Legeza and M. Reiher, *J. Chem. Theory Comput.*, 2013, 9, 2959–2973.
[4] K. Boguslawski, F. Real, P. Tecmer, C. Duperrouzel, A. S. P. Gomes, O. Legeza, P. W. Ayers and V. Vallet, *Phys. Chem. Chem. Phys.*, 2017, 19, 4317–4329.
[5] C. Duperrouzel, P. Tecmer, K. Boguslawski, G. Barcza, O. Legeza and P. W. Ayers, *Chem. Phys. Lett.*, 2015, 621, 160–164.

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