

CBC SEMINAR ANNOUNCEMENT



Professor Peifeng Su
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Recent progress for energy decomposition analysis

Energy decomposition analysis (EDA) is a useful tool for understanding the intermolecular interactions in the framework of quantum chemistry. In this talk, the recently developed LMO-EDA and EDA-PCM methods are presented. The LMO-EDA is an energy decomposition analysis for interactions in gas phase with HF or KS orbitals. Decomposing the total interaction energy into electrostatic, exchange, repulsion, polarization, and dispersion interaction terms, the LMO-EDA method is able to investigate nonbonding and bonding interactions with closed or open shell systems. The EDA-PCM method is a free energy decomposition scheme for analyzing the intermolecular interactions in various solvated environments based on LMO-EDA. In EDA-PCM, the solvated environment can be treated by CPCM, IEFPCM or Het-CPCM methods. The EDA-PCM is able to obtain the smooth curves of the total interaction energy and the individual EDA interaction terms in different dielectric environments along the whole potential energy surfaces. Test calculations show that the EDA-PCM is competent for various kinds of intermolecular interactions in various dielectric environments.

Bibliography

- (1) Su, P.; Li, H., *J. Chem. Phys.*, 2009, 131, 014102
- (2) Su, P.; Liu, H.; Wu, W. *J. Chem. Phys.* 2012, 137, 034111

Date:	20th December 2012 (Thursday)
Time:	2:30pm – 4:00pm
Venue:	NTU SPMS CBC Building Level 2, Conference Room
Host:	Asst Professor Hajime Hirao