NANYANG TECHNOLOGICAL UNIVERSITY

CBC SEMINAR ANNOUNCEMENT

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Recent Advances in Ab Initio Valence Bond Methods

In this talk, I would report some recent advances in the methodology developments of valence bond theory.[1] This talk will focus on the ab initio VB methods that are based on classical VB theory, which deal with purely localized orbitals and explicit consideration of covalent and ionic structures. Post-VBSCF methods, valence bond configuration interaction method (VBCI) and the valence bond second order perturbation method (VBPT2), will be reported in this talk. In the VBCI method, the VBSCF energy and wave function are improved by configuration interaction (CI). On the other hand, VBPT2 uses perturbation theory, taking the VBSCF wave function as the zeroth order reference. In addition, a hybrid method, called density functional valence bond (DFVB), is also discussed, which uses DFT to correct dynamic correlation to VB energy. Furthermore, several VB applications to the nature of chemical bonding are discussed.

Bibliography

Wu, W.; Su, P.; Sason, S.; Hiberty, P. C., *Chem. Rev.* 2011, 111, 7557-7593.

Date:	**20th December 2012 (Thursday)**
Time:	**11:00am – 12:30pm**
Venue:	**NTU SPMS CBC Building Level 2, Conference Room**
Host:	**Asst Professor Hajime Hirao**