Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

The Quantum Monte Carlo studies of Van der Waals interaction in bilayer systems[1] CHING-MING WEI, CHENG-RONG HSING, Institute of Atomic and Molecular Sciences, Academia Sinica, CHING CHENG, Department of Physics, National Cheng Kung University, CHUN-MING CHANG, Department of Physics, National Dong Hwa University — Van der Waals (vdW) interaction is one of the most fundamental physical quantities resulted from the quantum fluctuation of charges. However, it remains a challenge to account for this interaction quantitatively in both theory and experiment. For example, vdW interaction is one of the physical properties that the LDA and GGA of Density Functional Theory (DFT) fail to describe correctly. In recent years, there have been many proposals of DFT-vdW to overcome this deficiency. However, discrepancies in binding energy among these DFT-vdW results are usually apparent. In this talk, we present the Quantum Monte Carlo (QMC) and DFT studies of various bilayer systems: BN/BN [New. J. Phys. 16, 113015 (2014)], Silicene/Graphene, Silicene/BN and MoS2/Graphene. The calculations show large discrepancies among various DFT functionals. The QMC calculated binding energy was found to be larger than that obtained by the LDA calculation and smaller than those using DFT-vdW correction. Moreover, the QMC calculated interlayer interaction was found to have a longer-range behavior than all the available DFT schemes. The outcome of the present QMC study would provide a benchmark for future generation of various DFT XC functionals and guidance for prospective experiments.

[1]work supported by MOST, NCHC, NCTS and the Academia Sinica Computing Center of Taiwan.

Ching-Ming Wei
Institute of Atomic and Molecular Sciences, Academia Sinica

Date submitted: 14 Nov 2014 Electronic form version 1.4