Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

A TDLDA+U approach on strongly hybridized Frenkel excitons in Mott insulators and implications to TDDFT and GW+BSE[1] CHI-CHENG LEE, Academia Sinica, Taiwan, H.C. HSUEH, Tamkang University, Taiwan, WEI KU, Brookhaven National Laboratory — The applicability of nowadays first-principles approach on local excitations of strongly correlated systems is unknown. We therefore derived the dynamical linear response of LDA+U functional within the framework of TDDFT.[2] The strength and weakness of LDA+U functional in describing charge excitations of strongly interacting Mott insulators is examined via this TDLDA+U method. Formulated using real-space Wannier functions, a computationally inexpensive framework gives detailed insights into the formation of tightly bound Frenkel excitons with reasonable accuracy. Specifically, a strong hybridization of multiple excitons is found to significantly modify the exciton properties. Furthermore, our study exposes a significant generic limitation of adiabatic approximation in TDDFT with hybrid functionals and in existing Bethe-Salpeter-equation approaches, advocating the necessity of strongly energy-dependent kernels in future development. Finally, a superatom approach beyond TDLDA+U will also be discussed.

[1]This work is supported by DOE CMSN of USA, and NSC of Taiwan.
[2]Chi-Cheng Lee et al., Phys. Rev. B 82, 081106(R) (2010).

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Date submitted: 23 Dec 2010 Electronic form version 1.4