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Strong hybridization of Frenkel excitons in Mott insulators: a novel Wannier function perspective* CHI-CHENG LEE, Brookhaven National Laboratory, H. C. HSUEH, Tamkang University, WEI KU, Brookhaven National Laboratory — Linear response scheme of the time-dependent density-functional theory (TDDFT) has been quite successful in the study of the excitations of weakly correlated systems. However, its applicability to strongly correlated systems remains unclear, especially due to the poor quality of the exchange-correlation kernel essential for those systems. On the other hand, the local-density approximation + Hubbard U (LDA+U) approximation has been shown to describe quite successfully the ground-state properties and electronic band structures of Mott insulators. Therefore, it is timely to investigate the linear response of the LDA+U functional in the framework of TDDFT in describing excitations of strongly correlated systems. In this talk, a theoretical (diagrammatic) framework of the linear response of LDA+U (TDLDA+U) functional will be presented and applied to the study of Frenkel excitons in NiO within the first-principles Wannier basis. The advantages and disadvantages of LDA+U functional will be discussed, in comparison with more advanced many-body approaches. [1] B. C. Larson, et al. PRL 99, 026401 (2007)*Work supported by U.S. DOE - CMSN

Prefer Oral Session
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Tom Berlijn
tberlijn@gmail.com

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