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Local excitations in charge-transfer insulators: a super atom approach via Wannier functions[1] CHI-CHENG LEE, WEIGUO YIN, Brookhaven National Laboratory, WEI KU, Brookhaven National Laboratory and SUNY Stony Brook University — Local excitations in strongly correlated charge-transfer insulator are very often tied to the rich functionalities of these materials. However, these tightly bound local excitations prove to be difficult to calculate from first-principles. In particular, the strong local interactions render the typical first-principles perturbation approach (via diagrammatic Bethe-Salpeter equation) inapplicable to describe the multiplets. In this talk, our recent progress in evaluating the local excitations in NiO will be presented. Utilizing the gauge freedom of the Wannier functions, the oxygen (charge-transfer) degrees of freedom can be integrated into a "super atom", in which the strong local interactions can be incorporated on the equal footing as the strong coupling between the oxygen p- and Ni d- orbitals. Our results lead to good agreement with recent non-resonant inelastic X-ray scattering data [1] and the cluster calculation [2] for both q-dependence and excitation energies. Finally, extension to propagation of the local excitation will be addressed to include the dispersion in momentum space. [1] B. C. Larson et al, PRL 99, 026401 (2007) [2] M. W. Haverkort et al, PRL 99, 257401 (2007)

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