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Hybridization of local Frenkel excitons in strongly interacting NiO[1] WEI KU, CMPMSD, Brookhaven National Lab; Physics Department, State University of New York, Stony Brook, CHI-CHENG LEE, CMPMSD, Brookhaven National Lab; Physics Department, Tamkang University, Taiwan, R.O.C., HUNG-CHUNG J. HSUEH, Physics Department, Tamkang University, Taiwan, R.O.C. — Recent experimentally observed tightly bound excitons in NiO are explained by a newly developed linear response theory within LDA+U approximation. A novel picture of local Frenkel excitons naturally emerges from a real space formulation of exciton formation using the energy- resolved Wannier functions. Systematic analysis of microscopic interacting processes reveals that the large 1 eV splitting between the excitons is due to a strong hybridization between the Frenkel excitons via strong local interactions. Our new picture can be viewed as a simplest representation of the charge excitation involving complex multiplet structure in strongly correlated systems.

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