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Obtaining X-ray absorption near-edge structure for transition metal oxides via the Bethe-Salpeter equation YUFENG LIANG, Lawrence Berkeley National Lab, The Molecular Foundry, JOHN VINSON, National Institute of Standards and Technology, SRI PEMMARAJU, Lawrence Berkeley National Lab, The Molecular Foundry, ERIC SHIRLEY, National Institute of Standards and Technology, DAVID PRENDERGAST, Lawrence Berkeley National Lab, The Molecular Foundry — Transition metal oxides are an important class of materials featured with strongly correlated effects. Most interesting and yet to-be-unveiled physics is associated with the metal 3d orbitals, which can be probed by X-ray absorption near-edge spectroscopy. A thorough interpretation of the x-ray spectroscopy is often accompanied with first-principles simulations of structures, electronic properties and the corresponding x-ray spectra. However, the simulation for TMOs is particularly challenging with the localized 3d orbitals. Most previous studies relied on the ground-state calculations without the core-hole as a compromise. Other treated the excited atom as a charged impurity but the calculated spectra turn out to be even more deviated from experiments [1]. Here, we present the first study for the O K-edge for several typical TMOs via solving the Bethe-Salpeter equation (BSE). We have found that electron-core-hole interactions can alter the absorption spectra significantly. Our study helps to disentangle core-hole effects from the intrinsic electron correlations and hence facilitates the development of more advanced many-electron theories. [1] Isao Tanaka, Teruyasu Mizoguchi, and Tomoyuki Yamamoto J. Am. Ceram. Soc., 88 [8] 20132029 (2005)

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