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The electronic structure of thorium halides predicted by HSE and GW JASON ELLIS, XIAODONG WEN, RICHARD MARTIN, Los Alamos National Laboratory — Recently, there has been a significant experimental push to measuring the VUV nuclear excitation of ^{229}Th using optical spectroscopy. Large band gap Thorium halides such as ThF_4 and Na_2ThF_6 have been suggested as candidate materials for studying this nuclear transition, as they are transparent to the relevant optical frequencies. In this work, we compare the many body GW approach, hybrid density functional theory, and local density approximation calculations of the electronic structure of these materials, as well as the rest of the binary thorium halides (ThX_4, X=Cl,Br,I).

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