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Electronic and optical properties of a metal-organic framework with ab initio many-body perturbation theory[1] KRISTIAN BERLAND, Univ. of Oslo, Dept. Physics, SMN, KYUHO LEE, Lawrence Berkeley National Lab., Molecular Foundry , SAHAR SHARIFZADEH, Dept. of Electrical and Computer Engineering, Boston University, JEFFREY B. NEATON, Dept. of Physics, UC Berkeley — With their unprecedented surface area, and their structural and chemical tunability, metal-organic frameworks (MOFs) are being thoroughly explored for applications related to gas storage. Less studied are their electronic, excited-state, and optical properties. Here we explored such properties of Mg-MOF-74 using a combination of density functional theory (DFT) and many-body perturbation theory (MBPT) within the GW approximation and the Bethe-Salpeter equation (BSE) approach. The near-gap electronic conduction states were found to fall into two distinct categories: molecular-like and 1d-dispersive. Further, using the BSE approach, we predict a strongly anisotropic absorption spectrum, which we link to the nature of its strongly-bound excitons. Our calculations are found to be in good agreement with experimental absorption spectra, validating our theoretical approach.

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