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Electronic and optical excitations in building blocks of the metal organic framework MOF-5[1] BIN SHI, University of Illinois at Chicago, LINDA HUNG, TANER YILDIRIM, National Institute of Standards and Technology, SERDAR OGUT, University of Illinois at Chicago — Metal organic frameworks (MOFs) are a relatively new class of materials which are made of metal-oxide clusters linked by organic bridging ligands. In recent years, MOFs have received considerable attention due to their widely tunable structural, chemical and physical properties. We investigate one of the well characterized MOFs, MOF-5, whose framework consists of tetrahedral $[Zn_40]^{6+}$ units linked by rigid arylcarboxylate ligands. We use many-body perturbation (GW+BSE) and time-dependent DFT methods in real space to examine the electronic and optical excitations in the building blocks of MOF-5, such as $Zn_4O(COOH)_6$, basic zinc acetate $[Zn_4O(CH_3COO)_6]$, and tetranuclear zinc benzoate $[Zn_4O(C_6H_5COO)_6]$. The calculated spectra are compared with available experimental measurements and existing calculations to shed light on the controversy regarding the nature (metal-ligand versus ligand-ligand) of low-energy electronic and optical excitations in MOF-5.

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