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Rare-earth-based metal–organic frameworks with improved visible-light-harvesting properties: a quantum chemistry study

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ABSTRACT

This report proves that improving the visible-light-harvesting properties in rare-earth-based metal–organic frameworks (RE-MOFs) (labelled as RE–UiO-66, UiO = University of Oslo MOFs), with the aim of performing as potential visible-light-driven photocatalysts, is achievable. Thus, the design of MOFs with specific applications, especially those involving sunlight and material interactions, represents a growing field, which has been addressed in the herein work using quantum mechanical tools. We achieved to relate the light absorption properties with the structure in systems Y–UiO-66, Sc–UiO-66 and La–UiO-66, by evaluating the inclusion of well-known electron donor substituents in the structure of the 1,4-benzenedicarboxylate (BDC) linker (i.e. BDC-R, R: $–CH_3$, –OH, –SH and $–NH_2$). The electronic structure and optical properties of Y–UiO-66 were rigorously investigated using computational techniques combining molecular and periodic density functional theory (DFT) calculations. As a remarkable result, it was shown that including the groups –SH or $–NH_2$ in the BDC linker, induced a shift in the absorption bands to the visible region ($\geq$ 400 nm). Hence, a group of new RE-MOFs materials with optimal structural and photocatalytic properties is proposed. This

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