

Unveiling the optical and electronic properties of dimensionally confined halide perovskites with ab-initio simulations

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Metal halide perovskites are swiftly emerging as ideal candidates for opto-electronic applications. Their dimensionally confined analogues in particular present a broad range of functionalities, thanks to a unique set of features, like quantum confinement, enhanced many body interactions, formation of stable excitons, etc. Along with their unparalleled compositional flexibility, as related to the huge library of organic spacers available, these materials are becoming more and more interesting for technologic applications.

Here, we show how ab-initio simulations can contribute to build a sounded knowledge of the electronic and optical properties of these hybrid materials. We combine the ab-initio solution of the Bethe-Salpeter equation with detailed symmetry analysis to characterise the optical properties of these materials. Namely, we clearly assign the excitonic progression of these compounds, including the exciton fine structure and spin-properties, fully accounting for relativistic spin-orbit-coupling. Furthermore, we discuss the electronic properties of these materials, with special focus on the interactions in the out-of-plane direction, setting a sounded understanding based on simplified, symmetric models, then extending to a series of compounds reported experimentally.