

## Halide perovskites: recent advances in optoelectronic properties from atomic scale modelling.

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Both all inorganic and hybrid halide perovskites have undeniably remarkable characteristics for next-generation photovoltaics, which deserve to be better understood. There are many different perovskite structures that are currently widely explored as absorber materials among which 3D  $AMX_3$  and 2D  $A_2A'(n-1)M_nX_{(3n+1)}$  frameworks, where A, A' are cations, M is a metal, X is a halide. Here, through a couple of recent examples including newly discovered halide perovskite phases [1], we will discuss their optoelectronic properties based on first-principles calculations and semi-empirical modelling. Impact of interfaces [2], structural fluctuations [3], quantum and dielectric confinements [4] on charge carriers and excitons will be inspected. Particular attention will be paid on excitonic effects comparing the results of model calculations with low temperature optical spectroscopy and 60-Tesla magneto-absorption [5]. Theoretical inspection of low energy states associated with electronic states localized on the edges of the perovskite layers will also be shown to provide guidance for the design of new synthetic targets [6] taking advantage of experimentally determined elastic constants [7].

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