

Excitons in low-dimensional halide perovskites from first-principles calculations

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Abstract

Quasi-two-dimensional halide perovskites, with their layered structures and tunable properties, offer a rich platform for studying excitonic phenomena. Their anisotropic dielectric screening and charge-carrier masses favor strong exciton binding, but large unit cells have so far limited first-principles modelling. Recent advances in many-body perturbation theory, notably the *GW* and Bethe-Salpeter Equation approaches, now allow detailed, predictive simulations. This contribution presents microscopic insights into intra-, interlayer, and charge-transfer excitons, including their coupling to lattice vibrations, in quasi-2D halide perovskites. The results bridge theory and experiment, and enable targeted tuning of excitonic properties.