Composite approach for layered hybrid perovskites: band alignment, quantum and dielectric confinements

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Layered hybrid perovskites have recently re-emerged as potential technological viable solutions for photovoltaic and optoelectronic applications. Their environmental stability and immunity to moisture coupled to their exciting optoelectronic properties, have given them a new opportunity in the search of efficient solar cell and light emitting devices [1,2]. Understanding their fundamental optical and electronic properties will be important for optimization. To this aim, we present a systematic theoretical method that considers layered perovskites as composite materials in which band alignment between the perovskite and organic layers becomes affordable [3,4]. Such an alignment is an important performance criterion in the operation of optoelectronic devices. We investigate effects such as the thickness of the perovskite well, its chemical composition and the length of the organic barrier on the confinement potentials [4]. Moreover, we extend the method to inspect dielectric profiles with the salient feature of allowing the clear identification of the contributions of the perovskite and organic layers to the total dielectric profile [4]. Finally, with the insight gained from the different effects on band alignments, we propose design guidelines with the aim of achieving efficient optoelectronic devices. Hence, using the composite approach, we establish alternative theoretical methods to investigate the properties of layered perovskites and forecast that the approach will be relevant to inspect other 2D materials.

1) Tsai et al. “High-efficiency two-dimensional Ruddlesden–Popper perovskite solar cells” , *Nature*, 536, 312, **2016**
2) Mao et al., “Tunable White-Light Emission in Single-Cation-Templated Three- Layered 2D Perovskites $(CH_3CH_2NH_3)_4Pb_3Br_{10-x}Cl_x$”, *J. Am. Chem. Soc.*, 139, pp. 11956, **2017**
3) Even et al., “Understanding Quantum Confinement of Charge Carriers in Layered 2D Hybrid Perovskites”, *ChemPhysChem*, 15, 3733, **2014**
4) B. Traore et al., “Composite Nature of Layered Hybrid Perovskites: Assessment on Quantum and Dielectric Confinements and Band Alignment”, *ACS Nano*, 12, 3321, **2018**

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