Supporting Information

Excitonic and Polaronic Properties of 2D Hybrid Organic-Inorganic Perovskites

Jun Yin,[1,2] Hong Li,[1] Daniele Cortecchia,[3] Cesare Soci,[2] and Jean-Luc Brédas[1,]*

[1] Laboratory for Computational and Theoretical Chemistry of Advanced Materials, Division of Physical Science and Engineering, King Abdullah University of Science and Technology, Thuwal 23955-6900, Kingdom of Saudi Arabia

[2] Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link, Singapore 637371

[3] Energy Research Institute@NTU (ERI@N), Research Techno Plaza, Nanyang Technological University, 50 Nanyang Drive, Singapore 637553

Corresponding Author

jean-luc.bredas@kaust.edu.sa; jean-luc.bredas@chemistry.gatech.edu

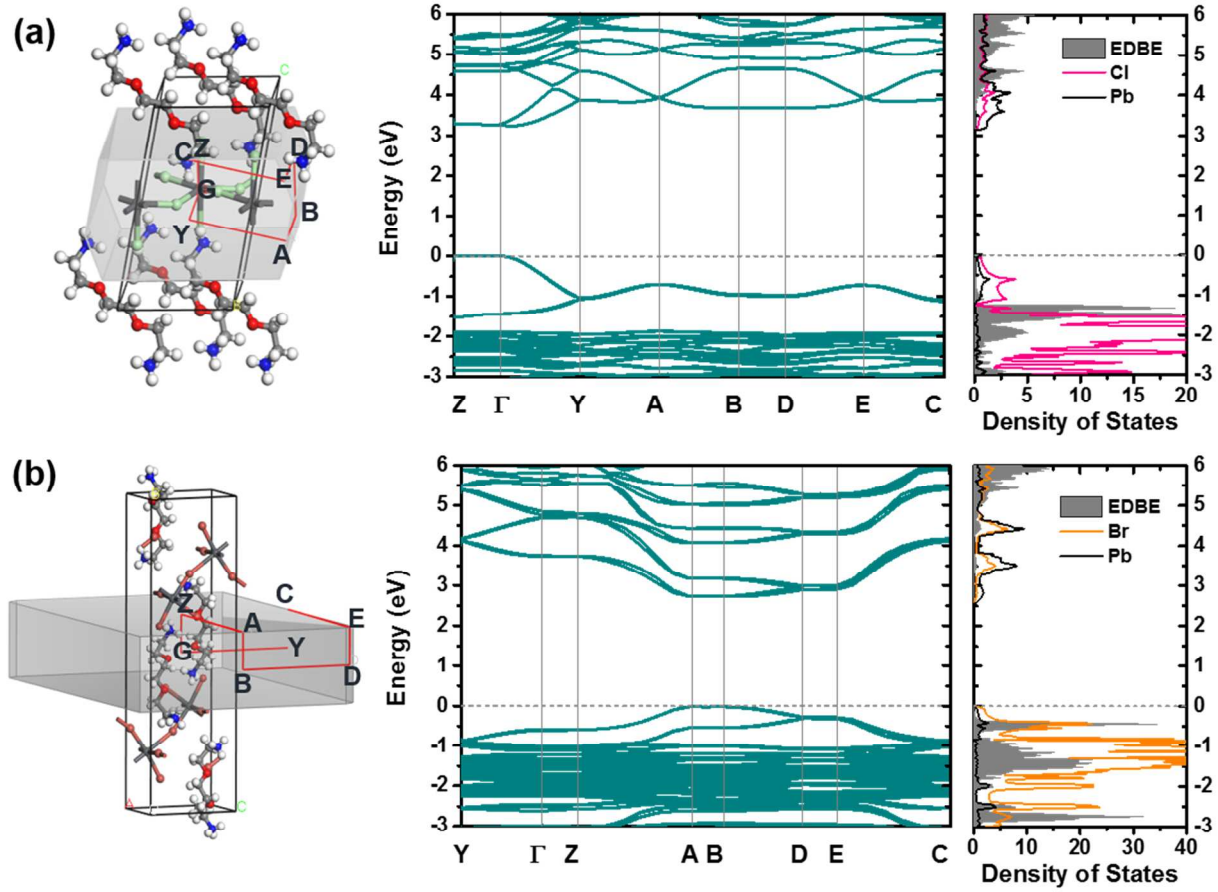

Figure S1. Band structures and densities of states of the two-dimensional perovskites: (a) (EDBE)$PbCl_4$ and (b) (EDBE)$PbBr_4$, calculated at the HSE+SOC level (VASP code).

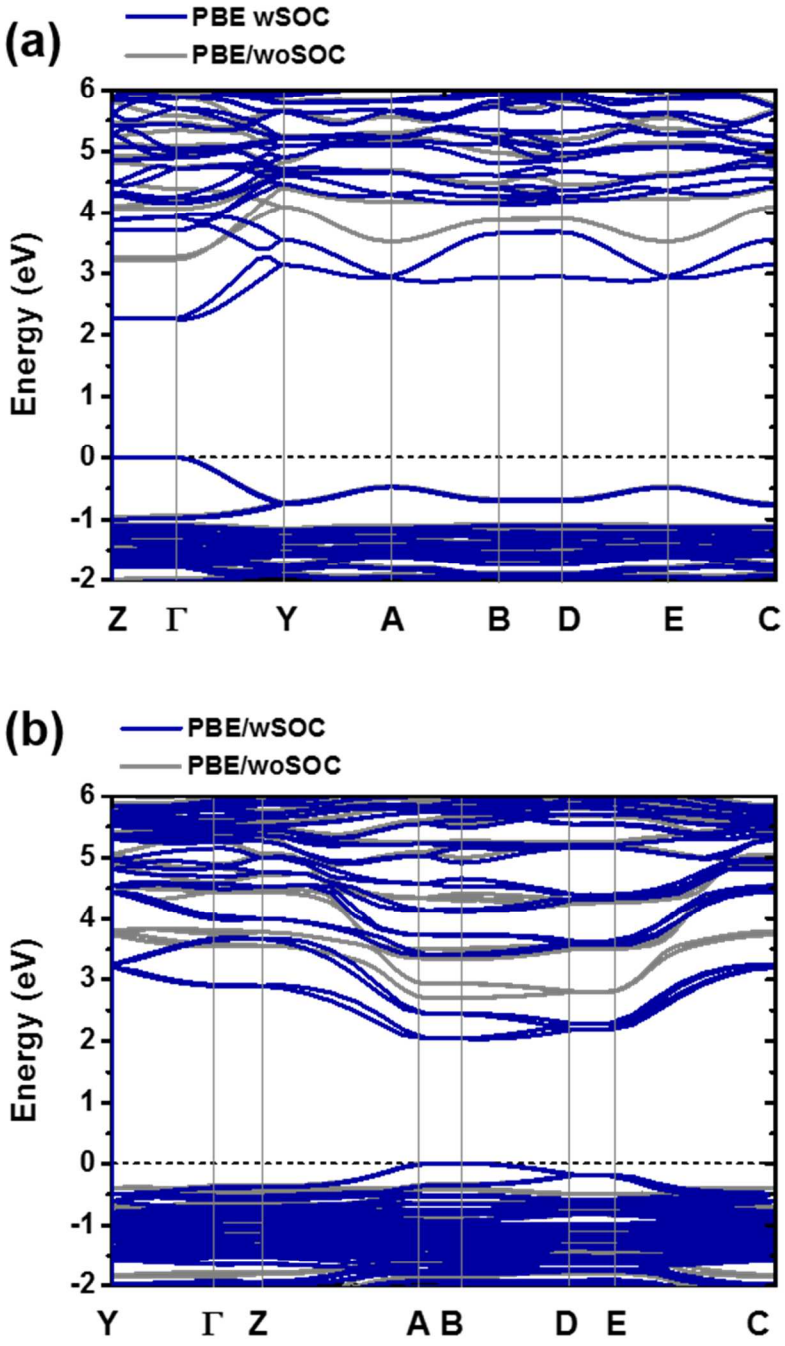

Figure S2. Band structures of the two-dimensional perovskites (a) (EDBE)$PbCl_4$ and (b) (EDBE)$PbBr_4$, calculated with and without consideration of spin-orbit coupling at the PBE level, used for the evaluation of the optical response (Quantum Espresso code).

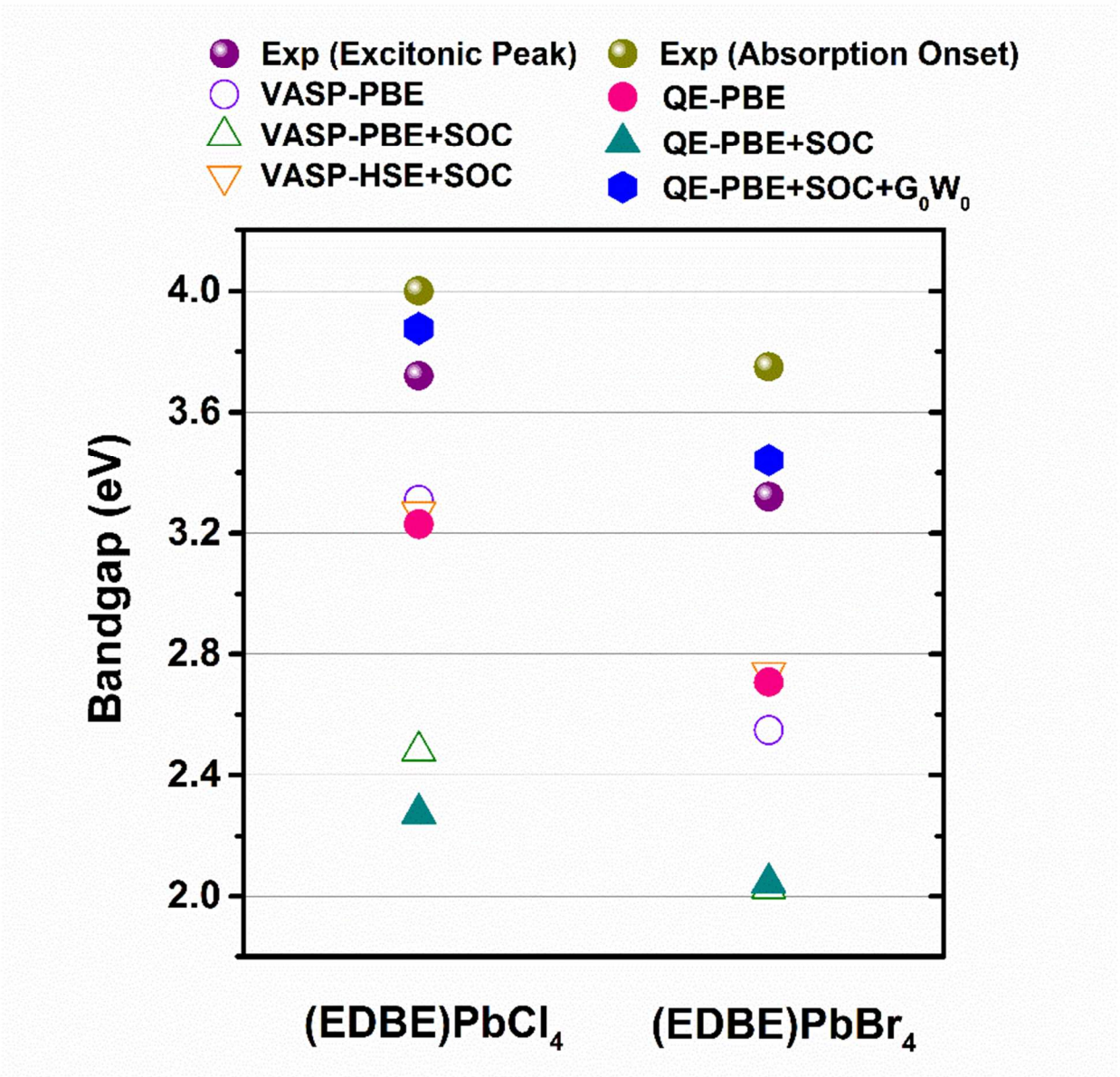

Figure S3. Bandgaps calculated using different methodologies (PBE, PBE+SOC, HSE+SOC, and PBE+SOC+G0W0) for the two-dimensional perovskites (EDBE)$PbCl_4$ and (EDBE)$PbBr_4$.

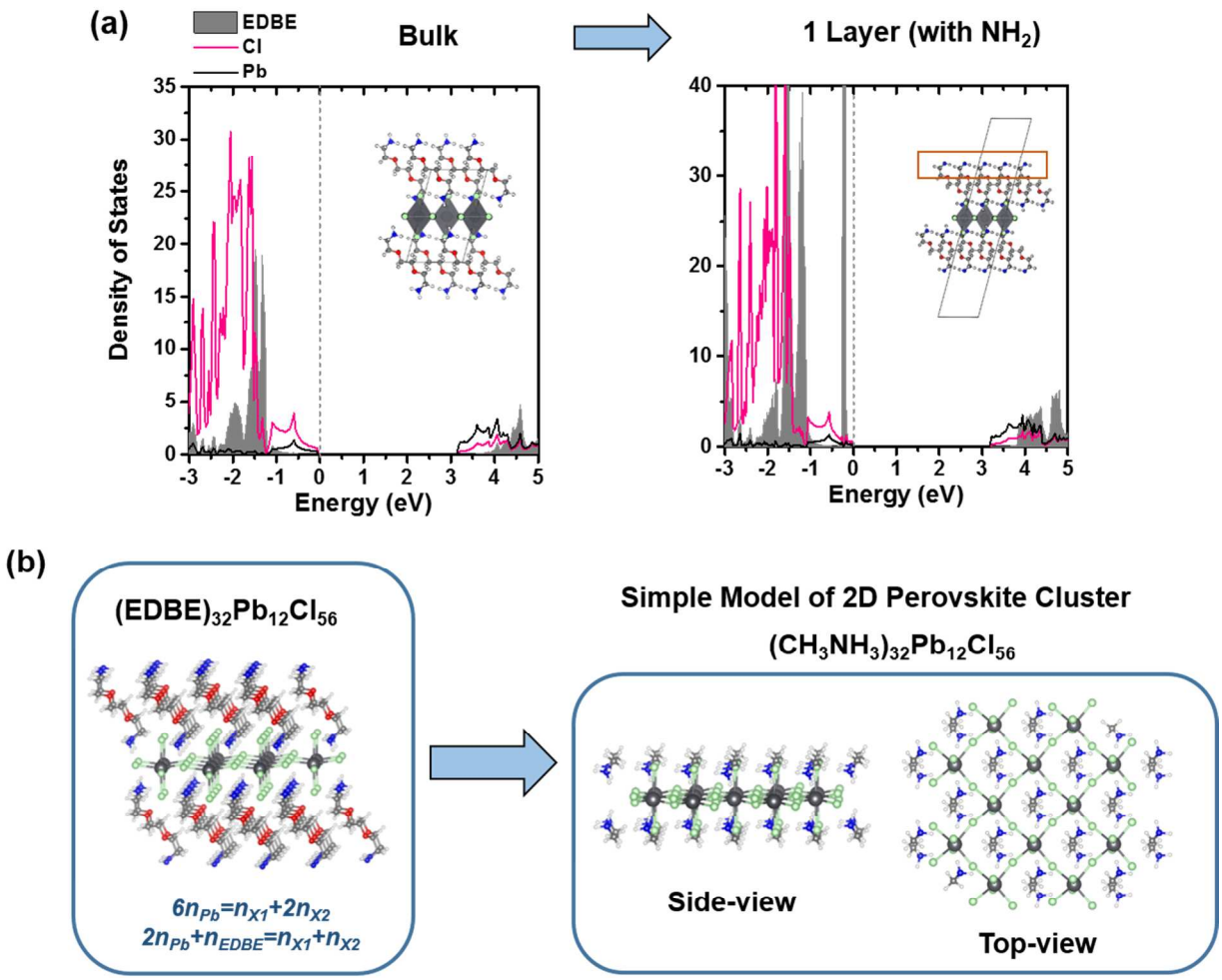

Figure S4. (a) Projected densities of states of (EDBE)$PbCl_4$ in the bulk and for a single layer with NH_2 terminations. (b) Molecular structures of the $(EDBE)_{32}Pb_{12}Cl_{56}$ cluster and corresponding simplified model of $(CH_3NH_3)_{32}Pb_{12}Cl_{56}$.