## Structural and optoelectronic properties of 2D multilayered perovskites and 2D/3D bilayers for photovoltaics

J. Even<sup>1</sup>, C. Katan<sup>2</sup>

## Univ Rennes, CNRS, Institut FOTON (Fonctions Optiques pour les Technologies de l'Information), UMR 6082, CNRS, INSA de Rennes, 35708 Rennes, France. Univ Rennes, ENSCR, INSA Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) -UMR 6226, F-35000 Rennes, France. jacky.even@insa-rennes.fr, claudine.katan@univ-rennes1.fr

2D multilayered metal halide perovskites share similarities with 3D perovskites including direct electronic band gap, sizeable optical absorption, small effective masses, Rashba-like effects [1]. They exhibit other attractive features related to tunable quantum and dielectric confinements, strong lattice anisotropy, more complex combinations of atomic orbitals and lattice dynamics, extensive chemical engineering possibilities, including chiral cations. This will be illustrated by recent combined experimental and theoretical studies on excitons, formation of edge states, hot carrier effects and carrier localization [2-7]. Moreover, combined in 2D/3D bilayer structures using new versatile growth methods, excellent solar cell device stability has been demonstrated [8]. The difference of performances between n-i-p or p-i-n device architecture can be rationalized based on band alignment calculations [9]. Noteworthy, the concept of lattice mismatch provides guidance for choosing the 2D and 3D materials to combine [10].

[1] J.-C. Blancon et al, Semiconductor physics of organic-inorganic 2D halide perovskites, Nature Nano.15 969 (2020)

[2] Y. Qin et al, Dangling octahedra enable edge states in 2D lead halide perovskites, Adv. Mat. 34, 2201666 (2022)

[3] W. Li et al, Light-activated interlayer contraction in two-dimensional perovskites for high-efficiency solar cells, Nature Nano, 17, 45 (2022)

[4] S. Cuthriell et al, Nonequilibrium Lattice Dynamics in Photoexcited 2D Perovskites, Adv. Mat. 34, 2202709 (2022)

[5] H. Zhang et al, Ultrafast relaxation of lattice distortion in two-dimensional perovskites, Nature Physics 19, 545 (2023)

[6] Quarti, C. et al., Exciton ground state fine structure and excited states landscape in layered halide perovskites from combined BSE simulations and symmetry analysis. Adv. Optical Mater. 2202801 (2023)

[7] S. Liu, et al, Bright Circularly-Polarized Photoluminescence in Chiral Layered Hybrid Lead-Halide Perovskites, Sci. Adv. 9, eadh5083(2023)

[8] S. Sidhik et al, Deterministic fabrication of 3D/2D perovskite bilayer stacks for durable and efficient solar cells, Science 377, 1425 (2022)

[9] B. Traore et al, A theoretical framework for microscopic surface and interface dipoles, work functions and valence band alignments in 2D and 3D halide perovskite heterostructures, ACS Energy Letters, 7, 349 (2022)

[10] M. Kepenekian et al, Concept of lattice mismatch and emergence of surface states in twodimensional hybrid perovskite quantum wells, Nanoletters (2018)

Acknowledgments: This work was supported by the European Union's Horizon 2020 research and innovation program under grant agreement 861985 (PeroCUBE). J.E. is supported by Institut Universitaire de France.