

Metal Halide Perovskites: A New Class of Semiconductors

C. Katan^{*1}, B. Traore,² M. Kepenekian,¹ L. Pedesseau,² J. Leveillee,³ A. Schleife,³ A. Neukirch,⁴ S. Tretiak,⁴ J.-C. Blancon,^{4,5} A. Mohite,^{4,5} C. Stoumpos,^{6,7} M. G. Kanatzidis⁶ and J. Even²

¹ Univ Rennes, ENSCR, INSA Rennes, CNRS, ISCR, Rennes, FRANCE.
claudine.katan@univ-rennes1.fr

² Univ Rennes, INSA Rennes, CNRS, Institut FOTON, Rennes, FRANCE.

³ Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, USA.

⁴ Los Alamos National Laboratory, Los Alamos, USA.

⁵ Department of Chemical and Biomolecular Engineering, Rice University, Houston, USA.

⁶ Department of Chemistry, Northwestern University, Evanston, USA.

⁷ Department of Materials Science and Technology, University of Crete, Heraklion, GR.

Abstract: Metal halide perovskites have recently demonstrated undeniably remarkable characteristics for a wide range of optoelectronic applications. The perovskite fever began with 3D hybrid perovskites of chemical formula AMX_3 , made of corner-sharing MX_6 with M a metal, X a halogen, and A a small organic cation. These perovskites have opened a route toward low-cost manufacture of solar cells while offering currently certified conversion efficiencies over 24%, at the level of the best known thin film technologies and not far from monocrystalline silicon. Since the initial breakthrough mid-2012, halide perovskites have attracted worldwide efforts from the scientific community leading to an extensive exploration of their structural versatility and an ever-growing diversity of composition with a revival of all inorganic metal halide perovskites. Currently, many different metal-halide networks are synthesized and their optoelectronic properties deserve to be unraveled. Among others, new compositions such as $A'_2A_{n-1}M_nX_{3n+1}$ afford layered structures with a controlled number of octahedra in the perovskite layer interspaced with larger organic cations A' for most. Here, through a couple of recent examples including newly discovered halide perovskite phases as well as experimental data from the early 90's, we will discuss their optoelectronic properties based on first-principles calculations, semi-empirical and empirical modelling. Differences between this class of perovskite materials and conventional semiconductors will be highlighted. Impact of composition and structural pattern on properties will be inspected, with particular emphasis on the effect of quantum and dielectric confinements on charge carriers and excitons. Opportunities to further engineer halide perovskite properties will also be tackled in the prospect to provide guidance for the design of new synthetic targets.