Hybrid Organic-Inorganic Halide Perovskites: Dimensionality vs. Applicability. A Theoretical Standpoint

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Organic-inorganic halide perovskites (OIHPs) are compounds characterized by the AMX_3 stoichiometry (A=organic cation; M= Ge, Sn, Pb; X= halide) whose hybrid nature is conferred by the presence of organic cations that fit the semiconductor network cavities according to established tolerance size parameters [1]. The interest for 3D OIHPs stems from their superior features as light harvester in photovoltaic (PV) devices due to a wide range of unique properties [2]. From the very first assembled perovskite based cells [3] characterized by photoconversion efficiencies (PCEs) of ~3.5%, impressive breakthroughs have been achieved, leading to devices with PCEs that pass 22% [4]. In such context, methylammonium lead iodide ($MAPbI_3$, $MA={}^{+}CH_3NH_3$, see Fig. 1) is the most widely employed OIHP due to its high compatibility with solution-based processing, a high absorption coefficient, and a bandgap close to the optimal one for single junction solar cells. Nonetheless OIHPs characterized by the presence of other cations find applicability in solar cells [5].

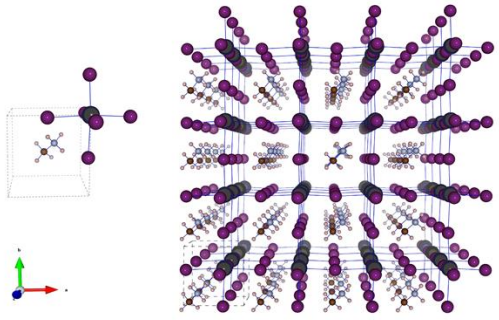

Figure 1: Optimized structure for (pseudo)-cubic $MAPbI_3$. Left: unit cell. Right: 4x4x4 supercell. (Reprinted with permission from Ref.[2e]. Copyright 2016 American Chemical Society).

While OIHP bulk (3D) properties have been massively investigated as testified by the huge number of papers recently appeared in literature, there is scarce knowledge of the chemico-physical properties of OIHP low-dimensional systems. This is surprising if one considers, for example, the possible applications of OIHP clusters (0D, see Figure 2) not only in PV but also in lasing and as quantum emitters [6].

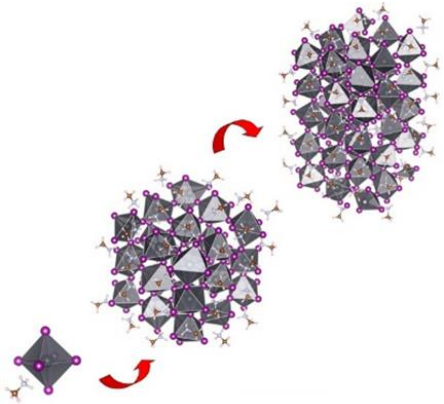

Figure 2: $MAPbI_3$ clusters of increasing size. (Reprinted with permission from Ref.[6b]. Copyright 2016 American Chemical Society.)

In the first part of this contribution I will provide an overview of the structural, electronic, and optical properties of 3D OIHPs, while the second part will mainly focus on results concerning, low-dimensional OIHPs, starting from 0D up to 2D systems, with particular focus on the chemistry and physics at the interface with transition metal oxides [7].

[1] (a) V. M. Goldschmidt, 1926 *Naturwissenschaften*, 14, 477; (b) G. Kieslich *et al*., 2014 *Chem. Sci*. 5, 4712.
[2] (a) J.-H. Heo *et al*., 2013 *Nature Photonics* 7, 486; (b) L. Etgar *et al*., 2012 *J. Am. Chem. Soc*. 134, 17396; (c) W. A. Laban *et al*., 2013 *Energy Environ. Sci.* 6 3249; (d) M. M. Lee *et al*., 2012 *Science* 338 643; (e) G. Giorgi *et al*., 2013 *J. Phys. Chem. Lett*. 4, 4213; (f) G. Xing *et al*., 2013 *Science* 342, 344; (g) S. D. Stranks *et al*., 2013 *Science* 342, 341.
[3] A. Kojima *et al*., 2009 *J. Am. Chem. Soc*. 131, 6050.
[4] http://www.nrel.gov/ncpv/images/efficiency_chart.jpg
[5] (a) A. Amat *et al*., 2014 *Nano Lett.* 14, 3608; (b) G. Giorgi *et al*., 2015 *J. Phys. Chem. C* 119, 4694 (Editor's choice).
[6] See for example (a) A. Fu *et al*., 2015 *Nature Materials*, 14, 557; (b) G. Giorgi *et al*. 2016 *J. Phys. Chem. Lett*., 7, 888, Perspective article
[7] G. Giorgi *et al*., *in preparation.*