Hybrid Organic-Inorganic Halide Perovskites: a novel class of materials for the renaissance of renewables. A theoretical standpoint.

Giacomo Giorgi
Dipartimento di Ingegneria Civile e Ambientale (DICA),
Università of Perugia, Via G. Duranti 93, I-06125 Perugia, Italia

Three dimensional organic-inorganic halide perovskites (OIHPs) are compounds with stoichiometric relation AMX_3 (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 well established tolerance size parameters.[1] The interest towards 3D OIHPs (2D OIHPs were already studied by David Mitzi at IBM for their possible optoelectronics applications[2]) derives from their superior features as light harvester in photovoltaic (PV) devices due to their manifold unique properties.[3] From the very first assembled perovskite based cells by Tom Miyasaka[4] in 2009 which were characterized by photoconversion efficiencies (PCEs) in the order of ~3.5%, impressive breakthroughs have been achieved, leading to devices with PCEs that nowadays are higher than 22%.[5] Methylammonium lead iodide ($MAPbI_3$, MA=$^+CH_3NH_3$) represents 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, even if OIHPs characterized by the presence of other cations may find applicability in solar cells.[6] OIHP bulk (3D) properties are nowadays receiving deep attention by the scientific community; at the same time there is total lack of knowledge of the chemico-physical properties of OIHP clusters and quantum dots (0D). This is astonishing because of their successful applicability in several devices, not only in PV but also in lasing and as quantum emitters.[7] In the first part of my talk I will provide an overview of the structural, electronic, and optical properties of bulk OIHPs, while the second part will mainly focus on results concerning 0D OIHP and also on the work in progress about interfaces and OIHP surface molecular passivation.

(1) (a) V. M. Goldschmidt, 1926 *Naturwissenschaften*, 14, 477; (b) G. Kieslich et al., 2014 *Chem. Sci.* 5, 4712.
(2) (a) D. B.Mitzi et al., 1995 *Science*, 267, 1473; (b) D. B. Mitzi, 2000 *Inorg. Chem.*, 39, 6107
(3) (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.
(4) A. Kojima et al., 2009 *J. Am. Chem. Soc.* 131, 6050.
(5) http://www.nrel.gov/ncpv/images/efficiency_chart.jpg
(6) (a) A. Amat et al., 2014 *Nano Lett.* 14, 3608; (b) G. Giorgi et al., 2015 *J. Phys. Chem. C* 119, 4694.
(7) 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; (c) G. Giorgi et al., 2016, *Phys. Chem. Chem. Phys*. 18, 27124.