

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Organic-inorganic hybrid lead iodide perovskite with zero-dipole-moment guanidinium ($\text{GA}=[\text{C}(\text{NH}_2)_3]^+$) cations: a Density Functional based analysis GIACOMO GIORGI, Department of Chemical System Engineering, The University of Tokyo, JUN-ICHI FUJISAWA, HIROSHI SEGAWA, Research Center for Advanced Science and Technology, The University of Tokyo, KOICHI YAMASHITA, Department of Chemical System Engineering, The University of Tokyo — Mixed organic-inorganic halide perovskites have been reported to have superior performances [1] and unique features [2, 3] when used as light harvesters in photovoltaics. Interestingly, they can undergo several assembling procedures like sensitization and thin-film architecture. The latter one has been anyway recently reported to be affected by a noticeable hysteresis in the $J - V$ curves at slow scan rate [4]. No conclusive reasons for such behaviour have been provided so far. By means of an *ab-initio* campaign of calculations [5], we predict possible chemical solutions based on the replacement of the widely employed methylammonium ($\text{MA}=\text{CH}_3\text{NH}_3^+$) cation with cations with reduced dipole moment, thus less sensitive to any applied external bias.

[1] Researchers at KRICT certified PCE of 17.9%.

[2] Xing et al., Science 342, 344 (2013); Stranks et al., Science 342, 341 (2013).

[3] Giorgi et al. J. Phys. Chem. Lett. 2013, 4 (24), pp 4213; J. Phys. Chem. C, 2014, 118 (23), 12176; J. Mater. Chem. A, (2014), DOI: 10.1039/c4ta05046k.

[4] Snaith et al., J. Phys. Chem. Lett., 2014, 5, 1511.

[5] www.vasp.at

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Date submitted: 13 Nov 2014

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