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The role of the methylammonium cation in the structural and electronic properties of 3D organic-inorganic perovskite halides: a DFT analysis including Spin Orbit Coupling GIACOMO GIORGI, Department of Chemical System Engineering, School of Engineering, The University of Tokyo, JUNICHI FUJISAWA, Research Center for Advanced Science and Technology (RCAST), The University of Tokyo & Japan Science and Technology Agency (JST), HIROSHI SEGAWA, Research Center for Advanced Science and Technology (RCAST), The University of Tokyo, KOICHI YAMASHITA, Department of Chemical System Engineering, School of Engineering, The University of Tokyo, RCAST & DEPARTMENT OF CHEMICAL SYSTEM ENGINEERING COLLABORATION — Many papers have been recently published reporting the enhanced photoconversion efficiency (PCE) up to 15% [Nature 501, 395 (2013)] for organic-inorganic solar cells containing sandwiches of perovskite compounds (the light harvester), mesoporous TiO_2, and a polymeric hole conductor. The usage of these 3D $MAPbX_3$ ($MA{=}CH_3NH_3^+$;$X{=}Cl^-$,Br,I^-) perovskites, stems by their chemical stability and good transport characteristics in the device. Anyway, these materials with so high applicability in PV and with many undisclosed features still find scarce attention in the theoretical community. Here, two aspects stimulated our work: the Spin Orbit Coupling (SOC) impact previously always speculated but ignored in predicting the electronic properties of these compounds, and the overlooked role played by the organic part. We focused on the electronic properties of $MAPbI_3$, on the impact played by SOC, on how hybrid functionals improve the bandgap prediction, and on the role ascribed to MA cation.

Giacomo Giorgi
Department of Chemical System Engineering,
School of Engineering, The University of Tokyo

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