Abstract Submitted
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Strain effects on the ferroelectric polarization of hybrid organic inorganic perovskite compounds SAURABH GHOSH, School of Applied and Engineering Physics, Cornell University, USA, DOMENICO DI SANTE, ALESSANDRO STROPPA, SILVIA PICOZZI, University of L'Aquila, Department of Physical and Chemical Sciences, Via Vetoio, L'Aquila and CNR-SPIN, Via Vetoio, L'Aquila, Italy, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University, USA — Metal-organic frameworks (MOFs) are hybrid crystalline compounds composed of an extended ordered network made up of organic molecules, organic linkers and metal cations. In particular, MOFs with the same topology as inorganic ABO_3 perovskites, have been shown to have interesting properties, *i.e.* coexistence of ferroelectric and magnetic ordering [1]. In this present work, using first-principles density-functional theory, we have investigated the effect of strain on previously reported MOFs, such as $C(NH_2)_3Cr(HCOO)_3$ and $(CH_3CH_2NH_3)Mn(HCOO)_3$. In these systems, a peculiar canted ordering of the organic A-cation dipole moments give rise to a *weak* ferroelectric polarization. We show that compressive strain can substantially increase the ferroelectric polarization, as much as 200%. Our study highlights the complex interplay between strain and dipole canting and put forward the possibility of tuning of ferroelectric polarization through appropriate thin film growing that can have potential applications in organic electronics.

[1] Stroppa, A.; Barone, P.; Jain, P.; Perez-Mato, J. M.; Picozzi, S. Advanced Materials 2013, **25**, 2284-2290.

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