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Engineering Multiferroicity in Perovskite MOFs

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Abstract:

This talk will focus on our current efforts to design new class of Metal Organic framework (MOF) materials showing multiferroicity. MOFs with ABX_3 perovskite structure are currently gaining increasing attention due to their multifunctional nature that includes properties such as magnetism, ferroelectricity - areas that have been traditionally dominated by inorganic compounds. The main advantages of magnetic MOFs, compared to inorganic compounds, is their diverse properties arise from the organic-inorganic duality that combines both merits of organic and inorganic elements within a single phase of materials. However, the MOFs synthesized so far show weak ferromagnetism and polarization. Also the critical temperatures are usually much lower than room temperature. These features have adverse implications on their applicability.

In this work, we propose a mixed metallic MOF of ABX_3 perovskite topology- $[C(NH_2)_3]Mn_{0.5}Cu_{0.5}[(HCOO)_3]$, which is a new multiferroic with strong ferromagnetism and with large ferroelectricity. We show that in the above mixed metal MOF, A-type magnetic order is the ground state leading to a huge magnetization of $2\mu_B/F.U$. I will also discuss about the origin of ferroelectricity and a giant enhancement of the polarization in this compound.

References:

- [1] Eerenstein, W., Mathur, N. D. & Scott, J. F. Nature, 2006, 442, 759–765.
- [2] Rogez, G., Viart, N. & Drillon, M. Angew. Chem. Int. Ed. Engl. 2010, 49, 1921–1923.
- [3] Stroppa, A. et al. Angew. Chem. Int. Ed. 2011, 50, 5847–5850.
- [4] Di Sante, D., Stroppa, A., Jain, P. & Picozzi, S. J. Am. Chem. Soc. 2013, 135, 18126–18130.
- [5] Tian, Y.; Stroppa, A.; Chai, Y.; Yan, L.; Wang, S.; Barone, P.; Picozzi, S.; Sun, Y. Sci. Rep. 2014, 4, 6062.