## Ferroelectricity and magnetoelectricity in hybrid organic-inorganic compounds

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Ferroelectric materials have a wide range of applications in device electronics. In the last decade, materials displaying the coexistence of two or more ferroic orders in the same material, i.e., multiferroicity, have attracted a lot of interest due to their potential applications in devices exploiting cross-coupling phenomena such as the magnetoelectric effect. Most of the known ferroelectric and multiferroic materials are inorganic compounds, being typically transition-metal oxides. However, in recent years the search for new multiferroic materials has been extended to hybrid organic-inorganic compounds such as metal-organic frameworks (MOFs) [1,2]. MOFs are porous crystalline compounds consisting of networks of metal ions connected by coordinating organic linkers, whose cavities can be filled by organic cations. Magnetism can be brought in by the metal framework, whereas novel functional properties can be tailored by suitably choosing the organic building blocks which enter the cavities. The hybrid character of MOFs, therefore, may lead to novel mechanisms by which ferroelectric, magnetic and magnetoelectric properties can be realized and tuned. In this respect, computational approaches based on density functional theory represent a valuable tool for identifying such mechanisms and for devising promising candidates in a material-design approach. Some representative examples in the class of MOFs with perovskite structure will be discussed, highlighting the role of organic cations and of their interplay with the metal framework in mediating ferroelectricity and magnetoelectricity [3-7].

## **References:**

[1] R. Ramesh, Nature 461, 1218 (2009).

[2] G. Rogez, N. Viart and M. Drillon, Angew. Chem. Int. Ed. 49, 1921 (2010).

[3] A. Stroppa, P. Jain, P. Barone, M. Marsman, J. M. Perez- Mato, A. K. Cheetham, H. W. Kroto and S. Picozzi, Angew. Chem. Int. Ed. 50, 5847 (2011).

[4] A. Stroppa, P. Barone, P. Jain, J. M. Perez-Mato and S. Picozzi, Adv. Mater. 25, 2284 (2013).

[5] D. Di Sante, A. Stroppa, P. Jain and S. Picozzi, J. Am. Chem. Soc. 135, 18126 (2013).

[6] Y. Tian, A. Stroppa, Y. Chai, L. Yan, S. Wang, P. Barone, S. Picozzi and Young Sun, Sci. Rep. 4, 6062 (2014).

[7] Y. Tian, A. Stroppa, Y. Chai, P. Barone, J. M. Perez-Mato, S. Picozzi and Y. Sun, Phys. Status Solidi RRL. doi: 10.1002/pssr.201409470 (2014)