Ferroelectricity and magnetism in hybrid organic-inorganic compounds

A talk by Alessandro Stroppa

CNR-SPIN L'Aquila, Italy

DATE / TIME: Monday, March 31st 2014, 04:00 p.m.
LOCATION: Ludwig Boltzmann Lecture Hall, ground floor, Strudlhofgasse 4, 1090 Vienna

Alessandro Stroppa| alessandro.stroppa@aquila.infn.it

Ferroelectric materials, whose spontaneous polarization can be switched by an external electric field, have a wide range of applications in device electronics. Recent discoveries of ferroelectricity in organic solids have been limited to some well-known polymer ferroelectrics or a few low molecular mass compounds. Computational approaches based on density functional theory represent a valuable tool in order to predict or suggest new organic ferroelectrics with large values of ferroelectric polarization. In particular, the modern theory of polarization is used and symmetry analysis gives an important help for gaining insights into the mechanisms responsible for the ferroelectric polarization. Here we will focus on the description of the ferroelectric and magnetic properties of complex organic-inorganic systems, such as metal-organic frameworks (MOFs). In particular, MOFs with a perovskite topology show promising new routes for the cohexistence of ferroelectricity and magnetism, i.e. multiferroicity.[1-5]

References:

[1] T. Besara, P. Jain, N. S. Dalal, P. L. Kuhns, A. P. Reyes, H. W. Kroto, A. K. Cheetham, Proc. Natl. Acad. Sci. USA 2011, 108, 6828.
[2] P. Jain , V. Ramachandran , R. J. Clark , H. D. Zhou , B. H. Toby,
N. S. Dalal , H. W. Kroto , A. K. Cheetham , J. Am. Chem. Soc. 2009,131, 13625.
[3] A. Stroppa , P. Jain , P. Barone , M. Marsman , J. M. Perez- Mato,
A. K. Cheetham , H. W. Kroto , S. Picozzi , Angew. Chem. Int. Ed. 2011, 50, 5847.
[4] A. Stroppa, P. Barone, P. Jain, J. M. Perez-Mato and S. Picozzi, Adv. Mater.,(2013) 25, 2284.
[5] D. Di Sante, A. Stroppa, P. Jain, S.Picozzi, J. Am. Chem. Soc., 2013, 135, 18126.