A collaboration between Shanghai University and CNR-SPIN (L'Aquila) reveals persistent spin-texture, for the first time in a layered hybrid perovskite system with strong spin-orbital coupling.

ACTIVITY C Innovative materials with strong interplay of spin orbital charge and topological degrees of freedom-2020

Persistent Spin-Texture and Ferroelectric Polarization in 2D Hybrid Perovskite Benzylammonium Lead-halide

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2D ferroelectric Hybrid Organic-Inorganic Perovskites (HOIPs) are gaining considerable attention with merits of effective light absorption in the broadband range, high photogenerated carrier yield, and high charge carrier injection efficiency.

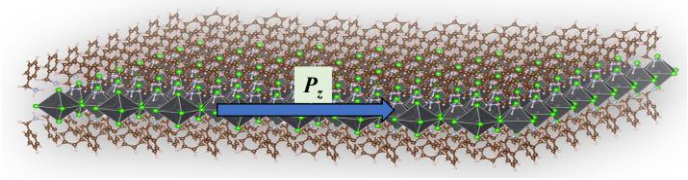

Fig. 1: The crystal structures of BA_2PbCl_4. There is an in-plane ferroelectric polarization in the system, in which organic molecules contribute 65% and inorganic frameworks contribute 35%.

In this work, a density functional study was performed on the electronic and ferroelectric properties of the bulk and monolayer benzylammonium lead-halide $(C_6H_5CH_2NH_3)_2PbCl_4$ which was firstly synthesized and characterized by Liao *et al* in Nat. Commun. 2015, 6, 7338. The calculations suggest that both the bulk and monolayer systems display a band gap of ~3.3 eV and a spontaneous polarization of ~5.4 μC/cm^2. The similar physical properties of bulk and monolayer systems support a strong decoupling among the layers in this hybrid organic-inorganic perovskite. Both the ferroelectricity, through associated structure distortion, and the spin-orbit coupling (SOC), through splitting induced in the electronic bands, significantly change the band gaps. Most importantly, for the first time in 2D hybrid organic-inorganic class of material, a peculiar spin texture topology was found, such as a unidirectional spin–orbit field, which may lead to a protection against spin-decoherence, thus supporting extraordinary long spin-lifetime of carriers, which is promising for spintronic applications.

This work is the result of the collaboration between Shanghai University and CNR-SPIN in L'Aquila. The first author Fanhao Jia is a PhD student of Shanghai University, Dr. Paolo Barone is a SPIN researcher providing a solid theoretical insight the spin texture. Prof. Wei Ren and Dr. Shunbo Hu of Shanghai University, and Dr. Alessandro Stroppa (SPIN) are the co-corresponding authors. The work has been published in The *Journal of Physical Chemistry Letters* (JPCL, Impact factor 2018: 7.329), a journal publishing "new and original experimental and theoretical basic research reporting a significant scientific advance and/or physical insight such that rapid publication is essential". The journal has dedicated the Supplementary Cover to this work (https://pubs.acs.org/toc/jpclcd/11/13).

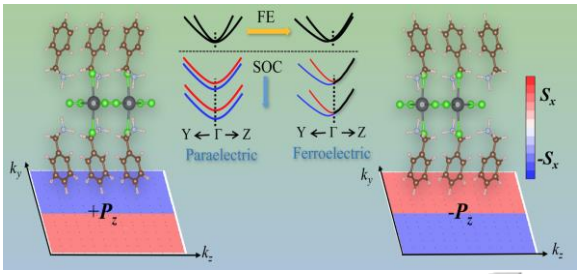

Fig. 2: The spin texture is indicated by the red and blue colors, which corresponds to the spin up or spin down along the out-of-plane *x* direction. The spin direction can be switched by ferroelectric polarization reversal. The unidirectional character of the spin texture tends to reduce the spin scattering, thereby leading to a protection against spin-decoherence. The inset is the band splitting of conduction band minimum due to SOC.