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Consiglio Nazionale delle Ricerche

Dear Editor,

We would like to bring to your attention our work entitled "Intertwined Rashba, Dirac and Weyl Fermions in Hexagonal Hyperferroelectrics" for consideration in Physical Review Letters.

As is well known, ferroelectrics can be in an electrically polarized state, either "up" or "down" oriented, and an external electric field is used to switch between these states. This makes ferroelectric materials appealing for novel technological applications. On the other hand, ferroelectrics suffer the well known problem of "depolarizing fields", especially in the thin-film limit. In fact, an internal electric field, called a depolarizing field, competes and usually destroys ferroelectricity when the system size is reduced below a few nanometers, i.e. the size needed for modern device applications. Hyperferroelectrics, however, have been demonstrated to sustain their polarization even in this ultra-thin film limit, making them promising materials for future thechnologies. [1-2]

Other appealing features that recently are gaining a lot of interest are those related to spin-orbit coupling (SOC). It has been proved that SOC is at the origin of many interesting phenomena in solid state physics, such as topological quantum phases and Rashba/Dresselhauss effects. All these phenomena play a leading role in the new field of spinorbitronics. [3] Furthermore, a non trivial interplay between ferroelectricity and SOC has been predicted to provide new functionalities, such as the electrical control of spin degrees of freedom. [4]

In this work, by means of first-principles calculations, we demonstrate that the newly proposed class of hexagonal hyperferroelectrics hosts an extremely rich variety of SOC-related properties, ranging from the electrical control of Rashba effects, to a nontrivial strong topological as well as Weyl-semimetal phases. We prove - by means of complementary approaches based on Bloch- and Wannier-functions, on "state of the art" DFT, on ab-initio tight-binding, and on the coherent potential approximation for disordered alloys - that such a rich physics is intimately linked to (hyper)ferroelectric properties, persisting even in the ultra-thin film limit

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and in an unscreened depolarization field. We believe that our findings, i.e., the link of relativistic properties and hyperferroelectricity, represent a major advance in the fields of new topological/Rashba materials as well as of relativistic ferroelectric semiconductors, paving the way for the electric control of SOC related functionalities in nanometer scale devices.

Your sincerely, the authors.

(D. Di Sante, P. Barone, A. Stroppa, K. Garrity, D. Vanderbilt, S. Picozzi)

References:

[1] K. F. Garrity, K. M. Rabe, and D. Vanderbilt, Phys. Rev. Lett. 112, 127601 (2014).

[2] N. A. Benedeck, and M. Stengel, Physics, Viewpoint: Polarization that Holds Steady.

[3] A. Hoffmann, and S. D. Bader, Phys. Rev. Applied 4, 047001 (2015) and references cited therein.

[4] S. Picozzi, Front. Physics 2, 10 (2014).

Below we report a list of possible expert referees that can help in reviewing our work.

1) Philippe Ghosez, University of Liége, philippe.ghosez@ulg.ac.be

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