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2012 SEMINAR SERIES PRESENTS

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Department of Physics and Astronomy

Prof. Serge Nakhmanson

Materials Science Division
Argonne National Laboratory, IL

Ab initio design of ferroic materials with advanced functionalities: 2D ferroelectricity and Goldstone-like modes in perovskite-oxide layers

With the help of first-principles-based computational techniques, we have recently predicted that Goldstone-like states (i.e., collective, close to zero frequency excitations of the system, requiring practically no consumption of energy [1]) can be artificially induced in a layered Ruddlesden-Popper [2] compound PbSr2Ti2O7, with polarization constrained to a plane [3]. Such excitations had been shown to exist in ferroelectric liquid crystals (which have very weak polarization) and some magnetic structures (as spin waves) but never before in "hard" polar materials. Their presence in oxide layers results in a variety of useful physical properties that include large, tunable dielectric constants and an ability to easily form polar vortices in a nanodot geometry. In a similar fashion to the well-known perovskite materials with morphotropic phase boundaries (MPBs), these states emerge as polarization rotations with almost no energy penalty, suggesting that the existence of an MPB is actually yet another manifestation of the Goldstone theorem in solids.

We elucidate the electronic-structure underpinnings of the Goldstone-like states in the perovskite-oxide layers by examining the properties of individual atomic planes and tracking their evolution as these planes are stacked together. In contrast with ferroelectric PbTiO3 that has no Goldstone-like excitations, their appearance in the layered structures is attributed to the breakdown of the network of cooperative pseudo Jahn-Teller distortions [4] on the Ti4+ sites, which leaves the Pb2+ site network in the PbO atomic planes as the primary source of the polar instability. We demonstrate that the lone electron pair activity of the Pb2+ sites and the presence of the bracing SrO planes are both paramount for the emergence of the Goldstone-like excitations, while the Ruddlesden-Popper structure, in principle, is not.

This project was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under contract No. DE-AC02-06CH11357.

References

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[2] S. N. Ruddlesden and P. Popper, Acta Crystallogr. 10, 538 (1957); 11, 54 (1958).
[3] S. M. Nakhmanson and I. Naumov, Phys. Rev. Lett. 104, 097601 (2010).
[4] I. B. Bersuker, Ferroelectrics, 164, 75 (1995); The Jahn-Teller Effect (Cambridge University Press, 2006).

Monday, June 4 - 4:00 pm
Room 136, Jorgensen Hall

Host:
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