北京大学量子材料科学中心

International Center for Quantum Materials, PKU

Weekly Seminar

Stabilization of highly polar $BiFeO_3$ like structure: a new interface design route for enhanced ferroelectricity in artificial perovskite superlattice

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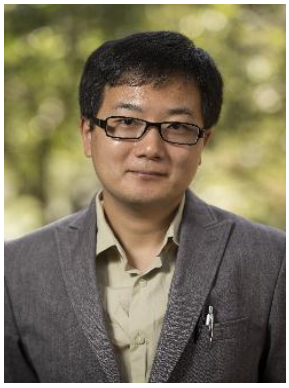

Time: 4:00pm, Dec. 28, 2016 (Wednesday)

时间：2016年12月28日 （周三）下午4:00

Venue: Room w563, Physics building, Peking University

地点：北京大学物理楼，西563会议室

Abstract

In ABO_3 perovskites, ferroelectricity is strongly coupled to oxygen octahedron rotations as a common structural distortion. However, this coupling behaves rather differently in various perovskite materials. It can promote large ferroelectricity in $BiFeO_3$ with *R3c* structure [1]. However, it suppresses ferroelectricity in $CaTiO_3$ with *Pbnm* symmetry [2]. For many $CaTiO_3$-like perovskite materials, the $BiFeO_3$ structure is a metastable phase. We report the stabilization of the highly-polar $BiFeO_3$-like phase of $CaTiO_3$ in the $BaTiO_3$/$CaTiO_3$ superlattice grown on a $SrTiO_3$ substrate. Stabilizing of this metastable phase is realized by a reconstruction of the oxygen octahedron rotations at the interface from the pattern in nonpolar bulk $CaTiO_3$ to a different pattern that is characteristic of a metastable $BiFeO_3$-like phase. This is shown through a combination of amplitude-contrast sub *0.1 nm* high-resolution transmission electron microscopy (HRTEM) and first-principles calculations of the structure, energetics, and polarization of the superlattice and its constituents. By demonstrating the predicted new artificial ferroelectric materials under this mechanism, we argue that a large number of perovskites with the $CaTiO_3$ structure type, which include many magnetic representatives, are now good candidates for novel highly-polar multiferroic materials [3].

References :

1. J. B. Neaton, C. Ederer, U. V. Waghmare, N. A. Spaldin and K. M. Rabe, First-principles study of spontaneous polarization in multiferroic BiFeO3, Phys. Rev. B **71**, 014113 (2005).
2. N. A. Benedek and C. Fennie, Why are there so few perovskite ferroelectrics, J. Phys. Chem. C **117**, 13339-13349 (2013).
3. N. A. Spaldin, S. W. Cheong and R. Ramesh, Multiferroics: Past, present, and future, Phys. Today **63**, 38 (2010).

About the speaker

Xifan Wu is currently a tenured associate professor at physics department of Temple University, he obtained BS degree in physics department of Nanjing University. He got his PhD degree in theoretical condensed matter physics in 2006 under the supervision of Professor David Vanderbilt from Rutgers University. He has been a postdoc research associate in Roberto Car's group at chemistry department of Princeton University. In 2010, he started the tenure track position in physics department of Temple University and was promoted to associate professor in 2016.