Prediction of a new multifunctional polar metal via first-principles high-throughput structure screening

Yue-Wen Fang[1,2*] and Hanghui Chen[2,3†]

[1]Department of Materials Science and Engineering, Kyoto University, Kyoto, Japan
[2]NYU-ECNU Institute of Physics, New York University Shanghai, Shanghai, China
[3]Department of Physics, New York University, New York, USA

Introduction

Polar metals–analogy of ferroelectrics in metals–are characterized by intrinsic conduction and inversion symmetry breaking. Polar metals are rare (especially in oxides) because mobile electrons screen electric fields in a metal and eliminate internal dipoles that are needed to break inversion symmetry. In this work, we use *ab initio* high-throughput structure screening to predict a new polar metal $BiPbTi_2O_6$ (BPTO) and demonstrate its potential multi-functions in electronic devices.

Lowest-lying bulk structures

Fig. 1 shows the lowest-lying structures from high-throughput screening, and the structural transitions under pressures and strains.

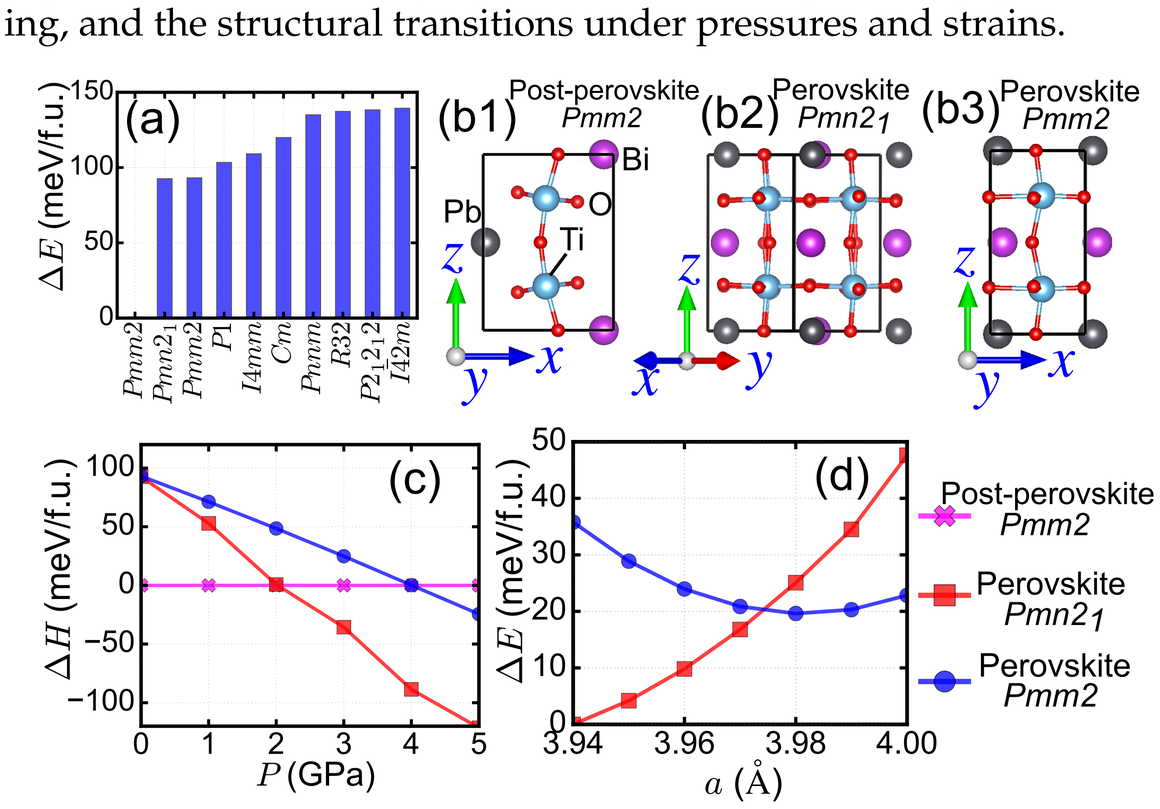

Fig. 1: **a** The ten lowest-energy structures of BPTO. **b1** Post-perovskite *Pmm*2; **b2** Perovskite $Pmn2_1$; **b3** Perovskite *Pmm*2. **c** Enthalpy (H) of the three lowest-energy structures under pressures. The H of post-perovskite *Pmm*2 is set as the zero point. **d** Total energy of the two lowest-energy perovskites as a function of epitaxial strain. The energy of perovskite $Pmn2_1$ constrained by $a = 3.94$ Å is chosen as the zero energy.

Electronic structures

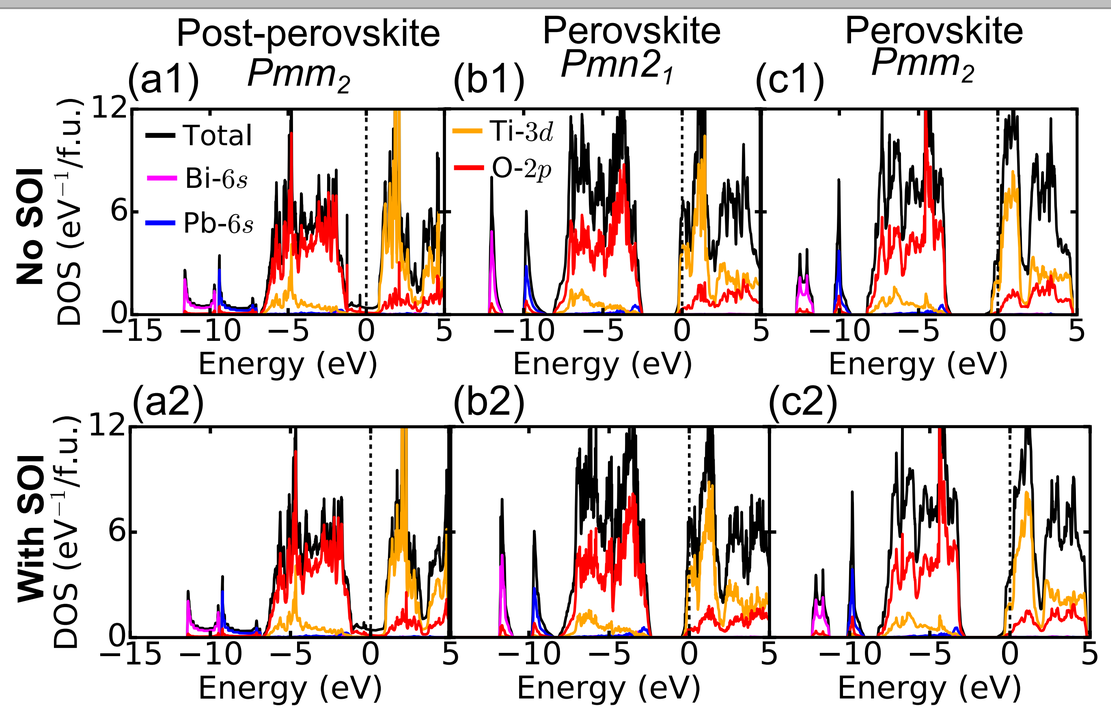

Fig. 2: Density of states (DOS) of BPTO of three polar structures calculated by DFT without spin-orbit interactions (upper panels) and DFT with spin-orbit interactions (lower panels).

References

[1] Yue-Wen Fang, Hanghui Chen, arXiv:1901.08771v2, 2019

Acknowledgements

We thank Kevin Garrity, Hongjun Xiang and T. Yamashita for valuable discussions. We acknowledge support from NSFC (No. 11774236), Pujiang Talents program (No. 17PJ1407300), the Seed Grants of NYU-ECNU Joint Research Institutes.

Nonpolar-polar transitions

Electron localization function (ELF) in Fig. 3 shows that a lobe-like lone-pair resides on one side of Bi and Pb ions in all three polar structures, which is the driving force to break inversion symmetry. The smooth energy curve indicates a continuous and spontaneous phase transition below a critical temperature.

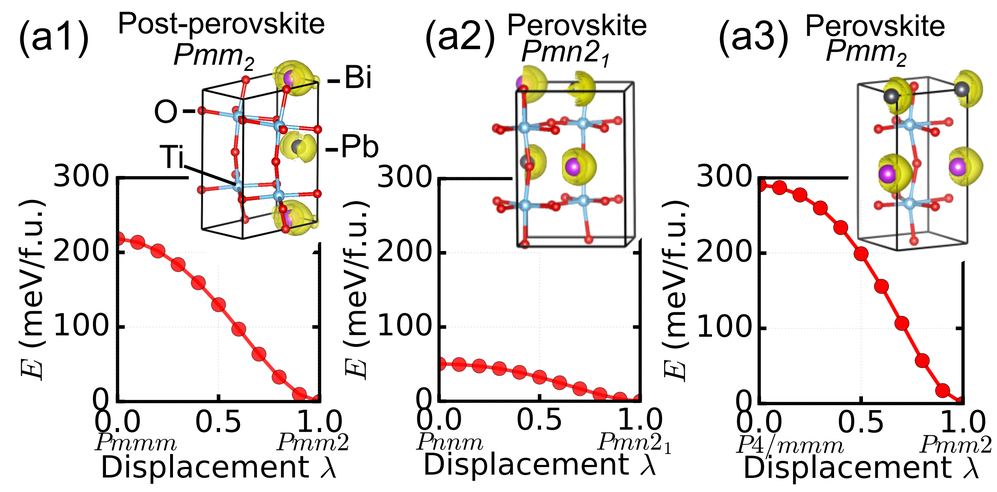

Fig. 3: The ELF and nonpolar-polar energy profile.

The switching barrier of BPTO thin film

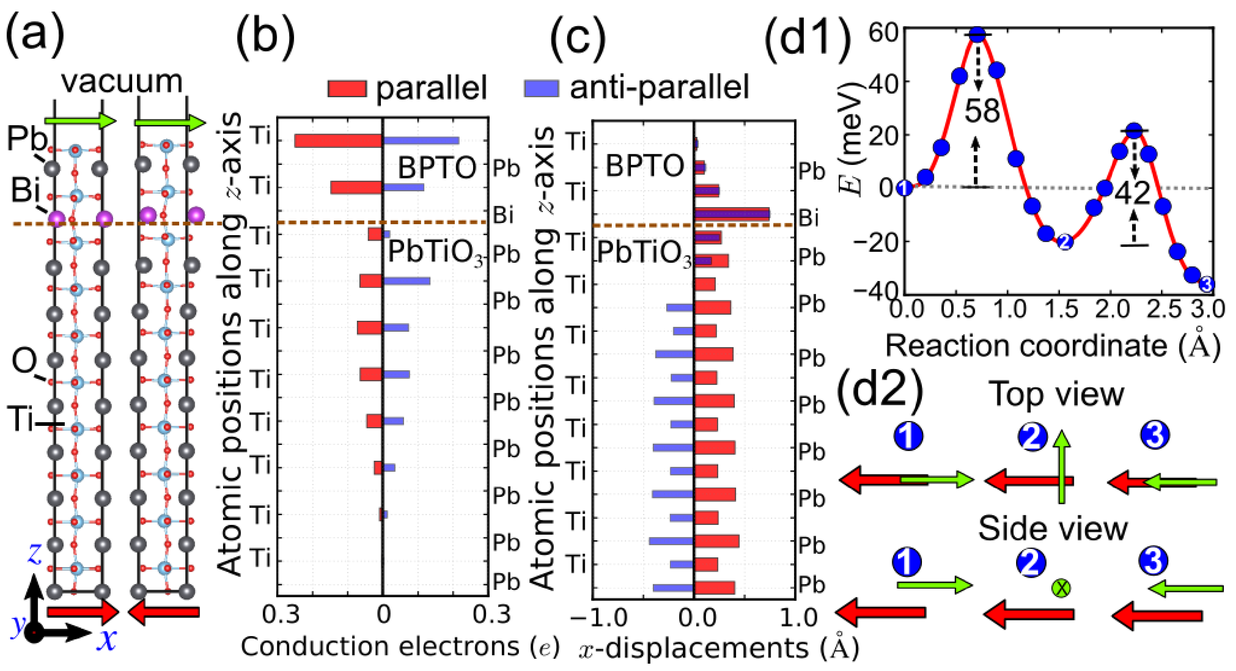

Fig. 4: **a** The "parallel state" (left) and "anti-parallel state" (right) of BPTO/$PbTiO_3$. **b** Layer-resolved conduction electrons on each Ti. **c** Layer-resolved polar displacements of metal ions. **d1** Calculated energy barrier. The three energy minima are schematically shown in **d2**.

Multifunctions of BPTO/PTO

In BPTO/$PbTiO_3$, at room temperature the interfacial coupling can overcome the switching barrier, which enables an electric field to first switch $PbTiO_3$ polarization and subsequently drive BPTO to 180° flip its polar displacements. At low temperature, an electric field can control $PbTiO_3$ polarization and stabilize multi states, implying different tunnelling resistance. This property can be used in multi-state memory.

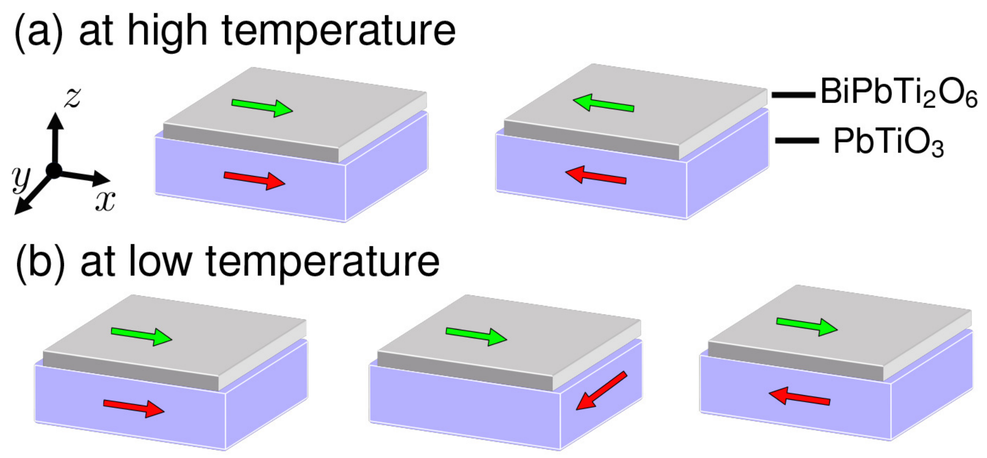

Fig. 5: Multifunctions of BPTO/PTO at **a** high and **b** low temperatures.

Conclusions

We demonstrate the power of first-principles high-throughput screening in designing new functional materials. In particular, we predict a new polar metal and propose its multi-functions in electronic devices.

Email: *fyuewen@gmail.com (Y.-W.F.) and †hanghui.chen@nyu.edu (H.C.)