Spin-textured ferroelectrics in InAs monolayer

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Abstract

Two-dimensional materials have attracted the attention for next-generation electronic devices [1]. With practical band gaps and high carrier mobilities, group III–V compounds have become a mainstream part of semiconductor research [2]. In the present work, the electric properties of InAs monolayer are investigated by *ab initio* calculations. Rashba and out-of-plane spin textures are respectively discovered around conduction band minimum (CBM) and valence band maximum (VBM), as shown in Fig. 1. A third-order $k \cdot p$ model of C_{3v} symmetry is presented to explain the mechanism [3]. Moreover, with a buckling structure, the properties of InAs are tunable by external electric fields (EEFs), as shown in Fig. 2. With EEF increasing from -0.5 to 0.5 V/Å, InAs remains to be a semiconductor. Meanwhile, both the structural buckling heights and Rashba constants are increasing, while the energy gaps are decreasing. More intriguingly, the switchable ferroelectricity has been verified in InAs. This work reveals the potential of InAs to be applied in spintronic, piezoelectric, and ferroelectric devices.

References

[1] Wu *et al.*, *Nature* **603**, (2022) 259–264.
[2] Alamo *et al.*, *Nature* **479**, (2011) 317–323.
[3] Miyamoto *et al.*, *Phys. Rev. B* **97**, (2018) 085433.

Figures

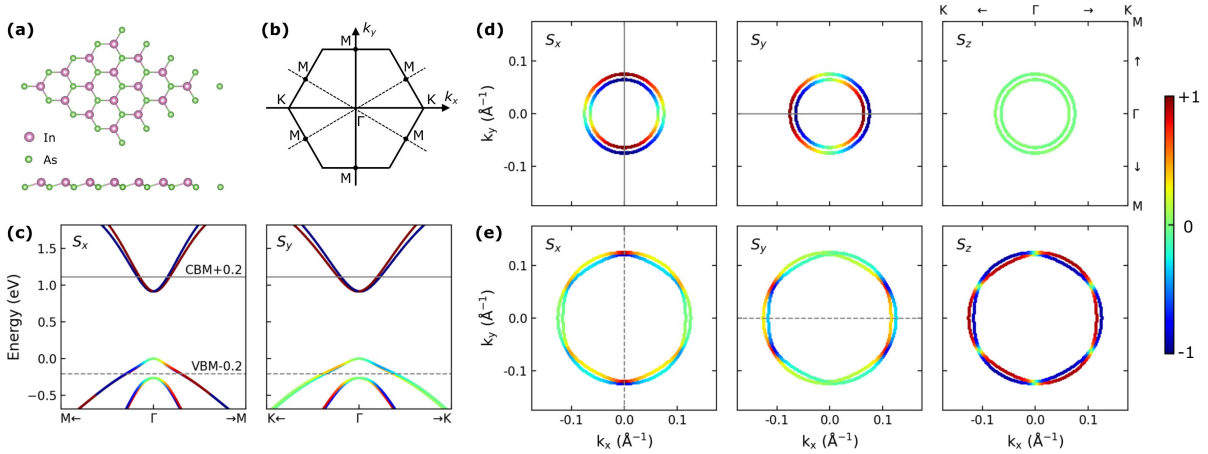

Figure 1: (a) Atomic structure of InAs monolayer (top view and side view). (b) Brillouin zone (BZ) and high-symmetry points. (c) Spin-resolved bands of S_x and S_y. Energy positions of CBM+0.2 eV and VBM-0.2 eV are marked by solid and dashed lines, respectively. (d) Spin textures in BZ at E = CBM+0.2 eV. (e) Spin textures in BZ at E = VBM-0.2 eV. The colorbar denotes the expectation values of spin operators.

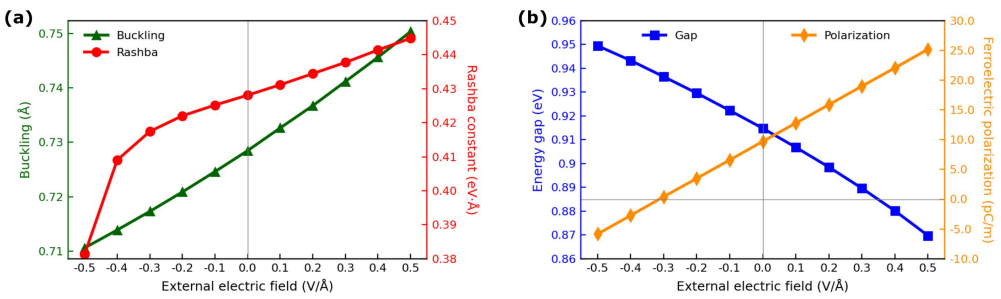

Figure 2: Tunabilities of InAs properties by EEFs: Buckling height, Rashba constant, energy gap, and ferroelectric polarization.