First-Principles Study of Doping Effects on Ferroelectricity and on Rashba Spin Splitting

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We investigates the effects of chemical and charge doping on ferroelectrics (PbTiO3 and BaTiO3) and the Rashba semiconductor (BiTeI). In the first project, we examined the polar instability and soft modes in electron-doped PbTiO3 using linear-response density functional calculations. We find that ferroelectric instability can sustain up to an electron concentration of n_e=0.7 per unit cell, surpassing the limits observed in LaAlO3/SrTiO3. Notably, electron doping transforms non-soft modes into soft modes, indicating a distinct microscopic mechanism for ferroelectricity in metallic states. Additionally, the frequency change $\Delta\omega/\Delta n_e$ remains remarkably flat at high doping levels, crucial for maintaining soft modes and polar distortion. We attribute this to strong mode-mode interactions, potentially extending the coexistence of metallicity and polar distortion.

In the second project, we explore Nb-doped PbTiO3 under various biaxial compressive strains to identify room temperature polar metals, essential for applications in superconductivity and magnetoelectricity. Our calculations show that at -2% and -3% strain, the A2u(TO1) polar mode exhibits stability under room temperature conditions, while unstrained Nb-doped PbTiO3 is unstable. Thus, strain significantly influences the properties of polar metals alongside doping.

Finally, we analyze the impact of electron and hole doping on the spin-orbit interaction and electron-phonon coupling in BiTeI. Our calculations reveal a maximum Rashba parameter of 7.46 eVÅ for the valence band and 6.32 eVÅ for the conduction band, the highest recorded to date. The electron-phonon coupling constant λ is found to be 0.46, similar to Al and Mo. However, the critical temperature (TC) of BiTeI remains low at 0.7 K, limiting practical applications.