Comparative first-principles studies of prototypical ferroelectric materials by LDA, GGA, and SCAN meta-GGA

Scientific Achievement

The performances of LDA, GGA, and SCAN meta-GGA for prototypical ferroelectric materials with diverse chemical bonds are analyzed and understood through comparative studies of various ferroelectric properties.

Significance and Impact

This work shows that the general-purpose SCAN functional significantly improves over LDA/GGA for simulating the structural, electric, and energetic properties of ferroelectric materials. SCAN significantly enhances the predictive power for ferroelectrics.

Research Details

Various well-known prototypical ferroelectric materials including perovskite systems ($BaTiO_3$, $PbTiO_3$, $LiNbO_3$), hydrogen-bonded systems (inorganic KH_2PO_4, organic PhMDA), and multiferroic systems ($BiFeO_3$, improper $YMnO_3$) are selected and their ferroelectric properties are studied. The performances of LDA, PBE, SCAN meta-GGA, and B1-WC hybrid functional are compared and explained.

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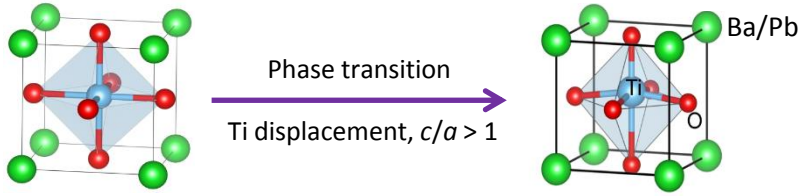
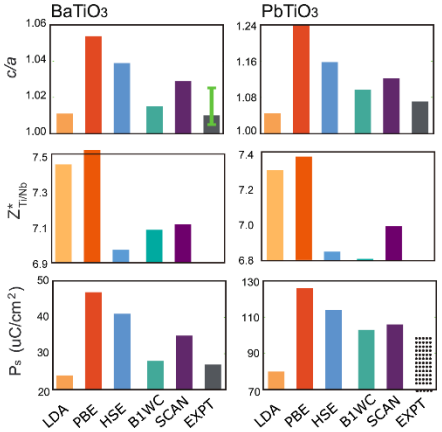
High-T Cubic structure, Paraelectric → Phase transition → **Low-T Tetragonal structure, Ferroelectric**

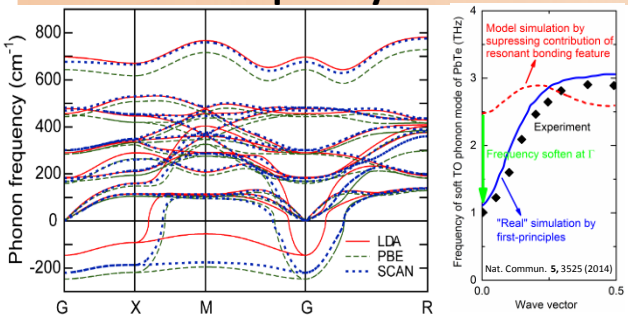


Fundamental ferroelectric properties



- Polar distortion c/a is underestimated by LDA, but is overestimated by PBE. Better prediction by SCAN
- Born effective charge Z^*, which is related to electronic polarizability, is overestimated by both LDA and PBE due to the **self-interaction error (SIE)**.
- c/a underestimation and Z^* overestimation by LDA result in **error cancellation** for predicting P_s. Better prediction by SCAN

Phonon frequency



- LDA: The good prediction of phonon frequency benefits from error cancellation (related to bonding strength & electronic polarizability)
- Reliable descriptions by SCAN

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