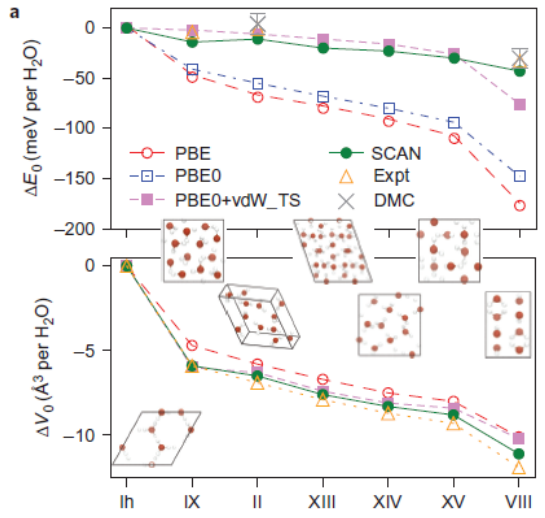
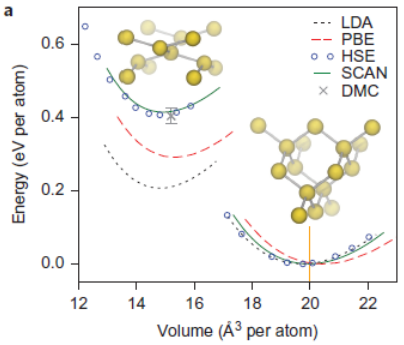
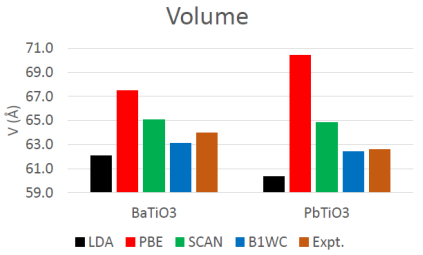
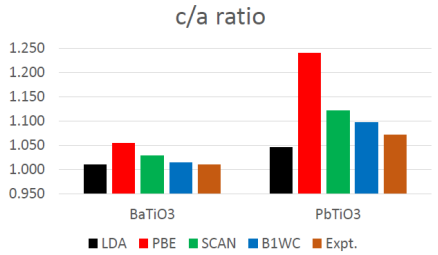
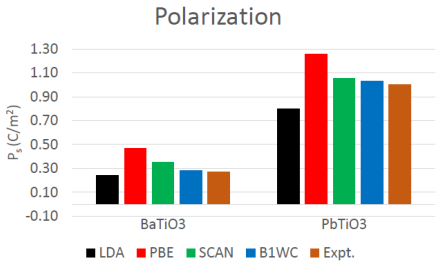
Accurate structures and energies of diversely bonded systems from an efficient density functional

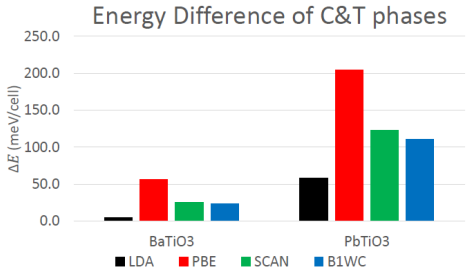












Up left: equilibrium volume and energy changes of 7 hydrogen ordered ice phases w.r.t the ground state ice Ih; **Up right**: energy difference between β-Sn and diamond phases; **Bottom**: properties of ferroelectrics, $BaTiO_3$ and $PbTiO_3$.

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Work performed at Temple University

Scientific Achievement

Accurate geometries and energies of diversely bonded systems were predicted by an efficient nonempirical semilocal density functional, the strongly-constrained and appropriately-normed (SCAN) meta-generalized gradient approximation.

Significance and Impact

Ground state potential energy surfaces are of great significance in chemistry, materials science, and condensed matter physics. This work establishes SCAN as an efficient functional that is accurate for various bonds (including covalent, metallic, ionic, hydrogen, and even van der Waals).

Research Details

Geometric and energetic properties of Si and H2O under different phases as well as ferroelectric materials were calculated. SCAN is overall significantly better than LDA and PBE for all tested systems. It is often comparable to, or even better than, computationally-expensive hybrid functionals (e.g., HSE and B1WC).

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