Semiconducting Ferroelectrics for Solar Energy Capture and Conversion

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We use first-principles density functional theory (DFT) calculations to investigate the ground-state structures of PbTiO3 solid solutions containing Ni, Pd, and Pt. Anomalous effective charges are reported, including the first report of negative Born effective charges for nominal +2 cations. We predict that these proposed materials will display a decreased band gap when compared to PbTiO3 while maintaining or enhancing polarization. They are promising candidates for use as semiconducting ferroelectric substrates for solar conversion devices.