Influence of vacancies on polarization and polarization switching from first-principles.

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We investigate the influence of vacancies on polarization and polarization switching in ferroelectric $BaTiO_3$ using first-principles calculations. Our study demonstrates that $BaTiO_3$ with V_{O1}^{2+}, V_{Ti}^{4-} and V_{Ba}^{2-} are insulators with nonzero electric polarization. Interestingly, we find that vacancy species have little effect on the polarization of $BaTiO_3$ as they produce polarizations comparable to that in perfect crystal. Furthermore, a new switching mechanism is proposed to reverse the polarization when vacancy is present. We show that the switching barrier in the presence of V_{O1}^{2+} is small with $\Delta E = 6$ meV per formula cell.