

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Ab initio polarization calculations for large systems using a Wannier center method OSCAR PAZ, KARIN M. RABE, DAVID VANDERBILT, Rutgers University — The ionic (\mathbf{P}_{ion}) and electronic (\mathbf{P}_e) terms in the electric polarization in solids are defined only modulo a quantum that connects different polarization branches and depends on the unit-cell dimensions. As the system cell size increases (especially perpendicular to \mathbf{P}) the quantum shrinks, becoming comparable to the expected polarization values, thus making the identification of the physically relevant branch unclear. To overcome this indeterminacy, a common approach involves multiple calculations of \mathbf{P} along an adiabatic insulating path, so that $\Delta\mathbf{P} \ll$ the quantum at every step. We remove the need for these multiple evaluations by using a representation of \mathbf{P}_e in terms of the centers of Wannier functions. In this intuitive picture, the arbitrariness in \mathbf{P}_e is removed by the implicit requirement that the position of the Wannier center move on a continuous path along with its corresponding ion or bond as the system is deformed from the initial to the final state. Our procedure for computing \mathbf{P} consists of associating each Wannier center with a particular atom or bond in the unit cell, and then obtaining \mathbf{P}_{ion} and \mathbf{P}_e through simple summations. We compare the results from this method to the Berry-phase technique using multiple evaluations for the case of supercell calculations of $V_{\text{Pb}}-V_{\text{O}}$ divacancies in PbTiO_3 . The same polarization values are obtained, with differences below $0.75 \mu\text{C}/\text{cm}^2$ associated with different k -point samplings.

Oscar Paz
Department of Physics & Astronomy, Rutgers University

Date submitted: 27 Nov 2009

Electronic form version 1.4