Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

**Efficient Computation of Spontaneous Polarization Using Wannier Center Displacements** JOHN BONINI, Rutgers University, OSCAR PAZ, ICM, Madrid, DAVID VANDERBILT, KARIN RABE, Rutgers University — A widely-used approach to computing the spontaneous polarization of a crystalline ferroelectric is to calculate the Berry-phase polarization for structures along a deformation path between the centrosymmetric and polar structures and use continuity of the polarization to resolve the ambiguity arising from the fact that the polarization of a bulk crystal is only defined modulo a lattice. In this work we formulate an alternative symmetry-based method to obtain the spontaneous polarization *using only one self-consistent calculation* by inferring the displacements of Wannier centers between oppositely polarized states. This method gives the same result as the first, while avoiding the inefficiency involved in construction of a deformation path and computation for multiple hypothetical structures. We present applications to a wide variety of ferroelectric structures. In addition, we will discuss how this formulation provides a natural framework for the physics of the switching polarization in more exotic cases, such as charge-ordered ferroelectrics.

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Date submitted: 11 Nov 2016 Electronic form version 1.4