Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Converse Piezoelectricity MICHAEL SPRINGBORG, University of Saarland, BERNARD KIRTMAN, University of California, Santa Barbara — Piezoelectricity results from a coupling between responses to mechanical and electric perturbations and leads to changes in the polarization due to strain or stress or, alternatively, the occurrence of strain as a function of an applied external, electrostatic field (i.e., converse piezoelectricity). Theoretical studies of those properties for extended systems require accordingly that their dipole moment or polarization can be calculated. However, whereas the definition of the operator for the dipole moment for any finite system is trivial, it is only within the last 2 decades that the expressions for the equivalent operator in the independent-particle approximation for the infinite and periodic system have been presented. Here, we demonstrate that the so called branch dependence of the polarization for the infinite, periodic system is related to physical observables in contrast to what often is assumed. This is related to the finding that converse piezoelectric properties depend both on the surfaces of the samples of interest even for samples with size well above the thermodynamic limit. However, we shall demonstrate that these properties can be calculated without explicitly taking the surfaces into account. Both the foundations and results for real system shall be presented.

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Date submitted: 01 Nov 2012 Electronic form version 1.4