THE UNIVERSITY OF CHICAGO

Computational and Applied Mathematics & Statistics Student Seminar

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Comparing ab initio methods to calculate polarization for high-throughput ferroelectric screening

TUESDAY,
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12:30 PM
Jones Laboratory,
Room 303

ABSTRACT

Ferroelectric materials exhibit spontaneous electric polarizations that can be tuned by external electric fields and have applications in information storage and electronic devices. While the polarization of a material can often be estimated using Born effective charges computed with density functional theory (DFT) and displacements relative to a nonpolar reference phase, prior high-throughput screening for candidate ferroelectric materials rely on the DFT-based Berry phase approach, accounting for the multivaluedness of the polarization by interpolating between the polar and nonpolar structures along a fictitious adiabatic path [1]. While this interpolation-based approach has identified new candidate ferroelectrics, it can fail to disambiguate branches or in cases where interpolated structures are spuriously metallic. Here, we compare these approaches with a recently proposed method, known as Berry flux diagonalization, which computes differences in Berry phase directly from the wavefunctions of polar and nonpolar structures, avoiding the calculation of the Berry phase polarization of multiple fictitious, interpolated structures [2]. Run times, accuracy, and limitations of these methods, with implications for high-throughput ferroelectric screening, will be discussed.

[1] Scientific data 7 (1), 1-22 (2020).
[2] Phys. Rev. B 102, 045141 (2020).
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