Unified Differentiable Learning of Materials Dielectric and Ferroelectric Responses

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Modelling material responses to external stimuli is a primary objective of computational materials science. However, current methods are limited to small-scale simulations due to the unfavorable scaling of computational costs. Here, we propose a machine-learning formulation where response properties stem from derivatives of a generalized potential function of atomic coordinates and applied external fields. Focusing on responses to electric fields, the method predicts electric enthalpy, forces, and dielectric responses within a unified equivariant model enforcing exact physical constraints, symmetries and conservation laws. Through application to α-SiO_2, we demonstrate that our approach can be used for predicting vibrational and dielectric properties of materials, and for conducting large-scale dynamics under arbitrary electric fields. We then apply our method to $BaTiO_3$ and determine the temperature-dependent ferroelectric hysteresis and the underlying dynamics of ferroelectric domains, thus going beyond the reach of standard quantum mechanical methods.

[1] S. Falletta, A. Cepellotti, A. Johansson, C. W. Tan, A. Musaelian, C. J. Owen, B. Kozinsky, arXiv:2403.17207 (2024)