MAR10-2010-020324

Abstract for an Invited Paper
for the MAR10 Meeting of
the American Physical Society

Ab initio construction of structure-property relationships in crystals

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While the cluster expansion formalism is traditionally used to parametrize the configurational-dependence of scalar properties (such as the total energy), this talk introduces a generalization of this widely used formalism to tensorial quantities (such as elastic constants, phase-transformation-induced strains, permanent dielectric dipoles, etc). This new method generates a suitable orthogonal basis for the space of all mappings from lattice configurations to tensors. It also provides symmetry rules to determine which terms in the Tensorial Cluster Expansion are equivalent by symmetry and must therefore share a common coefficient. The proposed framework encompasses, as special cases, a number of existing tools, including the local cluster expansion (used for modeling the properties of point defects), the "symmetrized" cluster expansions (used for predicting tensorial properties of disordered phases), and transferable force constants (used for efficient lattice dynamics calculations). This formalism also provides a simple language to describe the coupling between symmetry-breaking phase transformations and materials properties.