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Dielectric properties of solids in the regular and split charge equilibration formalisms RAZVAN NISTOR, MARTIN MÜSER, University of Western Ontario — We investigate the generic dielectric properties of solids in which atomic charges are assigned within the split-charge equilibration (SQE) method, which contains the regular charge equilibration method as a limiting case. It is shown that the latter always mimics ideal conductors, while any positive bond hardness, which is introduced in the SQE method, turns the solid into a dielectric. Crystals with simple cubic and rocksalt structure are considered explicitly. For these symmetries we map the split-charge formalism onto a continuum model, which can be solved analytically, e.g., we provide simple analytical expressions for how the dielectric constant and penetration depth depend on atomic hardness, bond hardness, and lattice constant. This mapping may prove useful when having to solve the dielectric response of a heterogeneous system to external electrical fields not only on the atomic but also on a coarse-grained scale. Successful comparison of numerical data to analytical solutions is made, including those that contain discretization corrections to the continuum solution.

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