The Electrostatics of Periodic Crystals

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Résumé

Madelung constants are indicators of the stability of crystal lattices. The convergence or divergence properties of the summations defining Madelung constants provide interesting mathematical challenges but also may relate to physical properties of the crystals. To study these properties, we utilize a concept commonly used in chemistry of a charge group made of the atoms in a crystal primitive cell. Charge groups that form an octopole (where the net charge, dipole moment, and quadrapole moment of the charge group vanish), such as for Na+–Cl– crystals, have the property that the corresponding contributions to the electrostatic potential can be summed in any order at least when the sums are done by charge groups. However, for charge groups with non-zero quadrapole moment, this is not the case. We show that a crystal primitive cell having 5 or fewer atoms must have a nonvanishing quadrapole moment. On the other hand, we show that for general charge groups with net charge zero and vanishing dipole moment, but nonzero quadrapole moment, it is possible to define a Madelung-like electric field. For charge groups of any type, we explain a plausible algorithm to define Madelung constants that uses a PDE framework and avoids questions of convergence of infinte sums. However, this framework leaves a certain (polynomial) ambiguity in the resulting electric field. We show that symmetries can reduce this ambiguity in many cases, but in important ones the ambiguity appears to be significant. More precisely, for charge groups with non-zero dipole moments, one can obtain what are called ferro-electric materials. For such materials, the order of summation clearly matters, as we show by simple examples using the abstraction of continuous dipole distributions. We derive other results regarding continuous dipole distributions, explaining several paradoxes.

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