

MACROSCOPIC ELECTROSTATICS AT POSITIVE TEMPERATURE FROM THE DENSITY FUNCTIONAL THEORY

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Density functional theory (DFT) has been a very successful effective theory of many-body quantum mechanics in the study of large molecules. In particular, the Kohn–Sham equations of DFT serve as an accurate descriptor of the electron density while limiting its computational complexity. One important class of electronic structures described by the Kohn–Sham equations is a crystalline lattice. At positive temperature, we show that a local perturbation to the crystalline structure induces an electric field governed by the Poisson equation. The latter equation emerges as an effective equation of the Kohn–Sham equations.