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Electric multipole interactions in an extended BEG model

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Abstract

General 2D dielectric phase diagrams and phase transitions for multipolar molecules adsorbed to a square ionic crystal are presented. The adsorbed molecules are modeled using a dilute spin-one Ising model in the Blume-Emery-Griffiths formalism, using a mean-field approximation. Physical constants such as the electric multipole moments and binding energies are used to uniquely determine the interaction parameters over the full range of physically-relevant values. We find that temperature- and coverage-dependent antiferroelectric to ferroelectric, coveragedependent ferroelectric up to ferroelectric down, reentrant ferroelectric to ferrielectric, and orderdisorder dipole phase transitions can occur. The results are presented as a quasi-continuous set of phase diagrams. Extensions into ferro-electric parameter space are discussed and connections to analytical solutions are explored.