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Simulation of structural phase transition in two dimensional ionic crystal[1] DONGSHENG ZHANG, GRAZIANO VERNIZZI, MONICA OLVERA DE LA CRUZ, Northwestern University — We investigate the structure of a two-dimensional monovalent ionic crystal observed in cationic-anionic molecules adsorbed into surfaces by molecular dynamics simulations. The pair interaction between ions include a short-range Lennard-Jones term and a long-range electrostatic term. When the dielectric constant is small, electrostatic interactions dominate and the crystal form a regular square lattice. At large values of the dielectric constant the Lennard-Jones attraction dominates, and the crystal form a triangular lattice. We study the phase diagram of this model and the properties of the structural transition.

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