Image method for Coulomb energy for many-body system of charged dielectric spheres JIAN QIN, JUAN DE PABLO, KARL FREED, University of Chicago — Ion polarization is important for understanding ion solvation and the stability of ion clusters in polymeric materials which typically exhibit a low and spatially inhomogeneous dielectric permittivity. The simplest approach for modeling ion polarization involves treating the ions as charged spheres with an internal dielectric permittivity differing from that of the medium. The surface polarization contribution to the electrostatic energy for a system of such dielectric spheres can be evaluated perturbatively. We derived closed-form expressions for this energy as a function of the positions of an arbitrary number of polarized surfaces. Our approach is a generalization of the image method for conducting spheres. Using this approach, we calculated the polarization corrections to the cohesion energy for ion clusters and for densely packed ionic crystals. The method can be readily adapted for investigating ion polarization effects in both Monte Carlo and molecular dynamics simulations.

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