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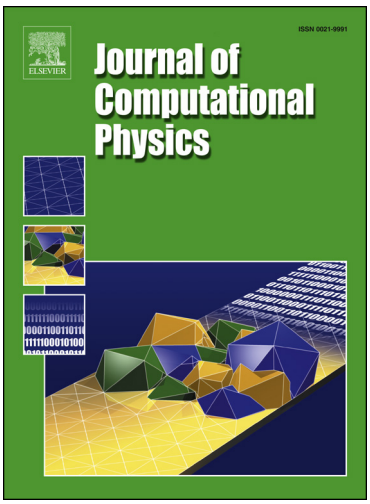

An integral equation approach to calculate electrostatic interactions in many-body dielectric systems

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Highlights

- numerically efficient solution to the problem of calculating electrostatic interactions between many dielectric particles is presented;
- the solution is general as it treats systems embedded in a homogeneous dielectric medium containing an arbitrary number of particles of any size, charge, dielectric constant and position in the three-dimensional space;
- the algorithmic complexity is reduced to linear scaling with respect to the number of particles;
- non-additivity of the electrostatic force in many-body systems is discussed;
- the effect of polarization at short separations on the total electrostatic force is considered for neutral – charged particle interactions, opposite charge and like charge interactions;
- the method is tested by the accurate estimations of the Madelung energy and constant of halite lattice;
- consequences for classical particle dynamics simulations are discussed.

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