



سمینار هفتگی ماده چگال نرم

Electrostatic Free Energy Computations for Solutions and Proteins

چکیده

Free energy calculation for solute with electrostatic charge requires special treatments based on the computational condition. Using periodic boundary conditions and different lattice sum methods for long-range interaction may change the real value of electrostatic potential calculated for the perturbing charged solute. In this infinite system, the electrostatic potential is conditionally convergent and dependent on computational conditions. In this talk, I will discuss the practical issues raised by electrostatic free energy calculations under various computational conditions, their origins, and possible solutions.

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