

Colloquium

PB-Steric Equations: A general model of PB equations

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摘 要：

Poisson-Boltzmann equation is a fundamental model for describing the distribution of ions. When ions are crowded, the effect of steric repulsion between ions (which can produce oscillations in charge density profiles) becomes significant and the conventional Poisson-Boltzmann equation, which treats ions as a point without volume, should be modified. Several modified PB equation were developed but the associated total ionic charge density has no oscillation. This motivates us to derive a general model of PB equations called the PB-steric equations with a parameter Λ , which not only include the conventional and modified PB equations but also have oscillatory total ionic charge density under different assumptions of steric effect and chemical potentials. As $\Lambda=0$, the PB-steric equation becomes the conventional PB equation but as $\Lambda>0$, the concentrations of ions and solvent molecules are determined by the Lambert type functions. To approach the modified PB equations, we study the asymptotic limit of PB-steric equations with the Robin boundary condition as Λ goes to infinity. Our theoretical results show that the PB-steric equations (for $0\leq\Lambda\leq\infty$) may include the conventional and modified PB equations. On the other hand, we use the PB-steric equations to find oscillatory total ionic charge density which cannot be obtained in the conventional and modified PB equations.

