سمینارهفتگی گروه ماده چگال نرم

Pores in lipid bilayers: Collapse and spontanous charging

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A continuum electrostatics theory is developed for ion-induced pore formation in lipid bilayers. The electrostatics of the polar head-group layer is included as a strongly anisotropic, high-dielectric layer covering the low-dielectric interior of the bilayers, as indicated by recent Molecular Dynamics simulations. Image-charge interactions produce a strong polarization attraction of the ion to the center of the pore, which reduces the electrostatic energy cost of pore creation. Depending on the value of the head-group dielectric constant, a pore may be water-filled – as in the existing transient pore model - or it may collapse, as reported by the Molecular Dynamics simulations. For sufficiently large head-group dielectric constants, the pore creation energy becomes negative with the ion losing its hydration shell. Instead, the trapped ion is surrounded by head-group molecular groups ("Born Trap"). The membrane charges spontaneously in this regime, by formation of arrays of pores, so neutral lipid bilayers would become self-repelling.

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