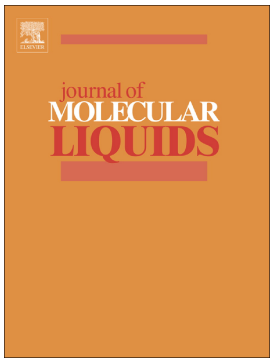

Influence of solvent granularity on the effective interactions between two overall neutral surfaces with quenched charge heterogeneity

Shiqi Zhou

PII: S0167-7322(18)33270-7
DOI: doi:10.1016/j.molliq.2018.09.138
Reference: MOLLIQ 9744

To appear in: *Journal of Molecular Liquids*

Received date: 27 June 2018
Revised date: 28 August 2018
Accepted date: 30 September 2018

Please cite this article as: Shiqi Zhou , Influence of solvent granularity on the effective interactions between two overall neutral surfaces with quenched charge heterogeneity. Molliq (2018), doi:10.1016/j.molliq.2018.09.138

* Corresponding author, Email: chixiayzsq@yahoo.com

Influence of Solvent Granularity on the Effective Interactions Between Two Overall Neutral Surfaces with Quenched Charge Heterogeneity

Shiqi Zhou

School of Physics and Electronics, Central South University,

Changsha, Hunan, 410083, China

Abstract: By using classical density functional theory of an electrolyte solvent primitive model (SPM), we investigate influences of solvent granularity on the effective interactions between two overall neutral planar surfaces with quenched charge heterogeneity over atomic length scale. Main conclusions are summarized as follows: (i) With consideration of the solvent granularity, the potential energy curves can (but not always) be highly oscillatory with a period approximately equal to the particle diameter. (ii) The present u_{elec}^{*} curve can change obviously with the bulk electrolyte concentration of the SPM in contrast with the homogeneously charged surfaces, but the concentration dependence of the u_{elec}^{*} curve will decrease as the charge separation extent decreases. (iii) Surface charge distributions, electrolyte types and bulk concentrations influence on the u_{elec}^{*} curve synergistically. For asymmetrical surface charge distributions, the electrolyte types and charge separation extent do not influence the overall u_{elec}^{*} curve shape evidently except that the first valley moves down with the electrolyte valency; by contrast, the overall morphologies of the u_{elec}^{*} curves for symmetrical surface charge distributions show features: first, for high valency salt and low bulk concentrations the u_{elec}^{*} is purely repulsive; only after the concentration becomes high enough, the alternating repulsive peaks and attractive valleys start appearing but still with weak strength. Second, in the presence of only low valency salt, the u_{elec}^{*} curves approximately as a whole (particularly the main valley) move up at low concentrations, and then move down at higher concentrations. Third, the concentration effect in the symmetrical surface charge distributions is not so obvious as that in the asymmetrical distributions. Using liquid theory arguments, all of these observations can be explained logically.

Key words: Solvent granularity; Effective electrostatic interaction; Quenched surface charge;