

Dissecting the Interactions of Superchaotropic Ions

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Polyoxometalates (POMs), among other large, multiply charged ions, associate with neutral polar surfaces, surfactants, and small nonionic molecules. [1] They favourably interact with nonionic surfactant foam [2] and micelles[3]. The unusual properties of these ions are explained by the “superchaotropic effect”. We have recently presented a classification of ions, which extends the Hofmeister scale and is based on ion size and charge [4]. However, many details of the molecular origin of this effect are not well understood.

Here we present all-atom and coarse-grained MD simulations of the interactions between $\text{PW}_{12}\text{O}_{40}^{3-}$ Keggin ions and oligoethylene glycoles. We quantify the interactions between Keggin ions and tetraethyleneglycol and between two Keggin ions by potentials of mean force and dissect the results into different contributions to the total free energy. Our results demonstrate the importance of contributions originating from water solvent, and help towards an understanding of the molecular driving forces of nanoion interactions.

Keywords:

Nanoions, Hofmeister effects, chaotropic effect

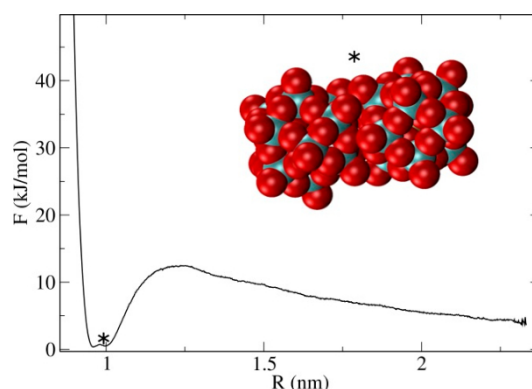


Figure 1: Potential of Mean Force between two Keggin ions from atomistic MD simulations. The snapshots shows a representative conformation of two ions at the distance of minimum free energy.

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