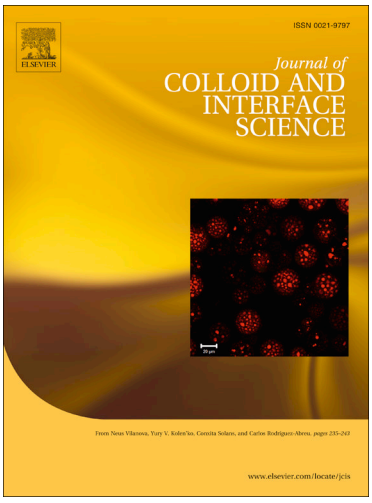

Regular Article

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Investigation of solvation of iron nanoclusters in ionic liquid $[N_{1114}][C_1SO_3]$ using molecular dynamics simulations: Effect of cluster size at different temperatures

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Abstract

The systems composed of metal nanoclusters in ionic liquids are relevant for applications in lubrication, electrochemical devices, catalysis, and chemical processes. The mechanism of solvation and interactions of these systems are not understood at present. In this work, we have simulated iron nanoclusters with different sizes in ionic liquid 1-butyl-1,1,1-trimethylammonium methane sulfonate $[N_{1114}][C_1SO_3]$ at two temperatures (300 and 500 K) and at atmospheric pressure. We have investigated the effects of cluster size and the temperature on some of the thermodynamics, structural and dynamical properties of the systems. Our results also show that the absolute value of solvation energy increases as the nanocluster size increases. Also the absolute solvation energy increases as the temperature increases. It is also shown that the effect of the cluster size is much more than the effect of the temperature. Our structural investigations indicate at least two shells (a double layer) around the nanocluster and the anions are closer to the cluster surface than the cations. The self-diffusion coefficients of cations, anions, and iron clusters have been also presented and discussed in this work.

Keywords: Solvation; Ionic liquid; Iron nanocluster; Molecular dynamics simulation.

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