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Effect of dissolved ions on dipolar correlations in liquid water UPAYAN BAUL, The Institute of Mathematical Sciences, C.I.T. Campus, Taramani, Chennai 600113, India, J. MARUTHI PRADEEP KANTH, Vectra LLC, 191, Hamid Building, Mount Road, Chennai 600006, India, RAMESH ANISHETTY, SATYAVANI VEMPARALA, The Institute of Mathematical Sciences, C.I.T. Campus, Taramani, Chennai 600113, India — Structural correlations in liquid water and the effect of dissolved ions on them have generally been characterized through short range density fluctuations. Recent simulation and experimental results have shown that there exists considerably longer ranged ($>$ 24 Angstroms) orientational order in water that can be studied using dipolar correlations. Using extensive molecular dynamics simulations, we show that the spatially long-range nature of such structural correlations are suppressed by the presence of ions, through reduction in co-operativity in orientational fluctuations. At high ($\geq$ 2M) concentrations, strongly solvated ions induce strong perturbations in the hydrogen bond network of water, leading to the formation of bulk like domains with defect sites on boundaries of such domains. Reorientational autocorrelation functions of dipole vectors of water molecules at such defect sites, which are beyond the first hydration shells of ions, also experience significant slowing of reorientation times. Our results show that the effect of ions on the properties of water can propagate well beyond the first solvation shells. Results are discussed in the context of hydrophobic effect and Hofmeister series.

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