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Abstract for an Invited Paper
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Dynamics in the First Hydration Shell of Anions¹

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We will describe our recent efforts to elucidate theoretically the vibrational and reorientation dynamics of water molecules in the first hydration shells of anions in aqueous solution, to assist in the interpretation of recent ultrafast infrared spectroscopic experiments on this issue. In particular, we will discuss (a) OH vibrational frequency dephasing for an iodide ion dilute in a solution of HOD in D₂O and (b) the reorientation dynamics for an HOD in the first hydration shell of a chloride ion dilute in a solution of HOD in D₂O. This work has been performed in collaboration with Damien Laage, Suyong Re and Bruno Nigro of the Dept. de Chimie, Ecole Normale Supérieure, Paris.

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