Soft X-ray Emission Spectroscopy of Water in Confined and Interfacial Conditions

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Water in nanoconfinement and at interfaces governs ion selectivity, charge generation, and electrochemical reactivity, yet its hydrogen-bond network is hard to probe under realistic conditions. O *K*-edge X-ray emission spectroscopy (XES) provides a direct fingerprint of water's valence electronic states, including $1b_1$-derived states sensitive to hydrogen-bond motifs. Here I present XES studies enabled by the BL07U HORNET-II station at NanoTerasu. A vacuum-isolation silicon nitride membrane allows measurements of wet interfaces while maintaining ultrahigh vacuum, with precise temperature/humidity control for well-defined adsorbed and confined water layers. Humidity-dependent XES tracks the evolution from molecular adsorption to water-cluster formation at polymer interfaces [1]. For liquid-crystalline polymer membranes showing strongly different rejection for mono- and divalent salts, XES identifies distinct stable water structures in nanopores that correlate with transport beyond pore size and fixed-charge effects [2–4]. I also discuss interfacial charge generation by ultrafine water clusters on self-assembled monolayers, where hydroxide-related signatures appear at both hydrophobic and hydrophilic interfaces [5]. These results highlight operando soft X-ray spectroscopy as a route to design rules for membranes and energy materials [6].

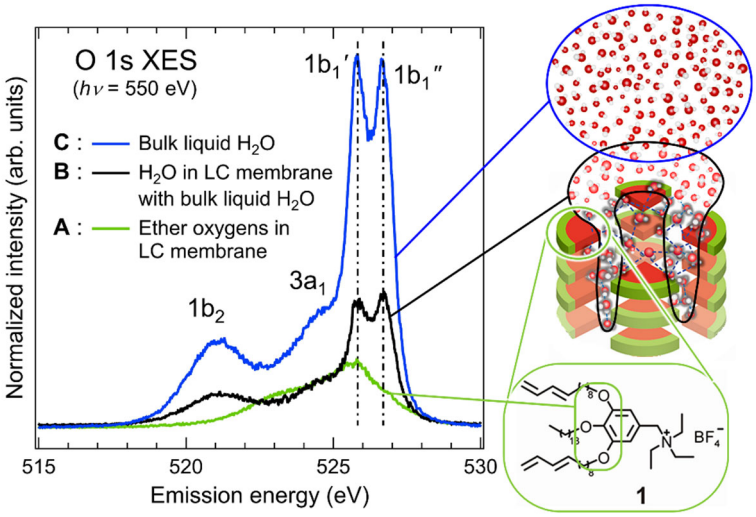

FIGURE 1. O 1s soft X-ray emission spectra indicate distinct water structures confined in nanopores of a liquid-crystalline polymer membrane, correlating with different salt rejection rates. Adapted from Ref. [4].

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