Two-dimensional hydration shells of alkali metal ions at a hydrophobic surface

SHENG MENG, DINKO V. CHAKAROV, BENGT KASEMO, SHIWU GAO, Department of Applied Physics, Chalmers University of Technology and Gothenburg University, SE-412 96 Gothenburg, Sweden — We study the hydration shell formation of alkali metal ions at a graphite surface. Two-dimensional (2D) shell structures are found in the initial stage of hydration, in contrast to the 3D structures in bulk water and clusters. Comparison of vibrational spectra with experiments identifies the shell structures and the thermally induced transition from the first to the second shell. We also found intriguing competition between hydration and ion-surface interaction, leading to different solvation dynamics between K and Na. Implications of these results in ionic processes at interfaces are elaborated.