הטכניון - מכון טכנולוגי לישראל

TECHNION - ISRAEL INSTITUTE OF TECHNOLOGY

הפקולטה להנדסה כימית
ע"ש וולפסון
The Wolfson Department of Chemical Engineering

Wolfson Department of Chemical Engineering Special Seminar
Lecture Hall 6, Wolfson Department of Chemical Engineering,
Wednesday August 28th 2019 at 1:30pm

Mr. Israel Zadok

Ph.D. candidate (advisors: Profs. Srebnik and Dekel)
Chemical Engineering – Technion

Unexpected hydroxide-water complex ion structure and properties at low hydration, understanding diffusion and stability in anion exchange membranes for hydrogen fuel cell applications

Hydroxide ion transport and structure in aqueous and non-aqueous media is fundamental to many chemical, biological and electrochemical processes. Research on hydroxide solvation behavior has primarily focused on a single fully solvated hydroxide, either as an isolated cluster or in the bulk. We discovered a new structure of water-hydroxide clusters that involve two hydroxides bridged by 2-3 water molecules. Such structures occur mostly in electrolyte systems involving cations with a large radius and at low hydration. These conditions can occur in anion exchange membranes for hydrogen fuel cells (AEMFCs), and may help shed light on their performance. Current engineering challenges in AEMFCs technology include overcoming low performance (diffusivity) and stability, both of which have been shown to be strongly correlated with hydration levels. We used molecular dynamics simulations and density functional theory to model several chemical systems at various hydration conditions, focusing diffusivity, hydrogen bond formation, and hydroxide-water complex statistics. The double hydroxide structures are shown to be more probable and more reactive at low hydration than the single hydroxides that dominate solvated conditions. We elucidate their effect on the hydrogen bond network in the hydrophilic phase and show that these newly observed double-hydroxide structures presumably disrupt the hydrogen bonded network required for structural diffusion of hydroxide ions through water. A simple model for the existence of these complexes is presented.

Refreshments will be served at 1:15pm