THANH-NGHI NGUYEN

will present his Ph.D. dissertation

Modeling of concentrated aqueous solutions of f-elements using a multiscale approach

The defense will take place on **Friday, December 4, 2015** at **2.00 pm**

in the ICSM Auditorium

Classical molecular dynamics simulations with explicit polarization have been successfully used to determine the structural and thermodynamic properties of binary aqueous solutions of uranyl chloride, perchlorate and nitrate (UO_2Cl_2, $UO_2(ClO_4)_2$ and $UO_2(NO_3)_2$). From a study performed as a function of the concentration of salts, the hydration properties of solutes and the ion-ion interactions of concentrated aqueous solutions of uranyl chloride, perchlorate and nitrate have been studied. The molecular dynamics simulations allow for reproducing the solvation properties of the hydrated uranyl, chloride, perchlorate and nitrate in good agreement with the experimental data. The results point out different coordination modes of Cl^- and ClO_4^- in the UO_2^{2+} second hydration shell and the presence of NO_3^- anion in the UO_2^{2+} first coordination shell at high concentration. The ion–ion interaction properties over water configurations have been studied at different concentrations.

Furthermore, we investigated the potential of mean force of ion pairs at infinite dilution as a function of the distance and the angle. The thermodynamical properties of the solutions have been calculated from these effective ion-ion pair potentials thanks to the McMillan–Mayer theory and molecular theory. The association constant of complex UO_2Cl^+ (K_{UO2Cl+}^{cal} = 2.52 L mol^{-1}), $UO_2ClO_4^+$ ($K_{UO2ClO4+}^{cal}$ = 2.34 L mol^{-1}) and $UO_2NO_3^+$ ($K_{UO2NO3+}^{cal}$ = 3.02 L mol^{-1}) has been determined and compared to the experimental ones. From the effective McMillan–Mayer potentials and using a multi-scale approach based on the MSA approximation, we also calculated the osmotic coefficients.

Keywords: Multiscale modeling; Molecular Dynamics; Uranyl; Electrolytes