

MOLECULAR DYNAMICS SIMULATIONS ON ION COMPLEXATION AND EXTRACTION: FROM CLASSICAL TO "GREEN" SOLVENTS

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Molecular dynamics simulations allow us to investigate at the microscopic level complex systems involved in cation complexation and extraction to classical, as well as non-conventional "green" solvents. The importance of interfacial phenomena will be highlighted, focusing on the extraction of lanthanide, actinide and Sr^{2+} cations. Examples involve (i) the uranyl extraction by TBP, diamides, BTP, dicarbollides, dithiophosphinic acids, and (ii) the effect of counterions in the Sr^{2+} extraction by crown ethers to supercritical CO_2 ¹. The evolution from well-defined interfaces to microemulsions will be described. Actinide and lanthanide ion solvation by room temperature ionic liquids will be presented.²⁻⁷

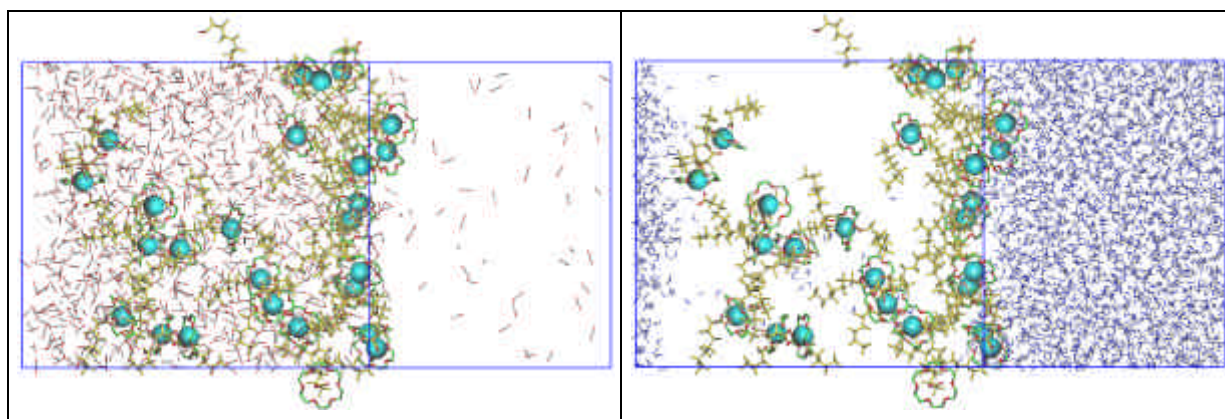


Figure: 25 $\text{Sr}\text{-}18\text{C}6(\text{PFO})_2$ complexes simulated at 350 K (with Ewald) at the CO_2 / water interface, showing an equilibrium between adsorbed and extracted complexes. Water and CO_2 solvents shown side by side instead of superposed for clarity.

(1) P. Vayssière and G. Wipff, *Phys. Chem. Chem. Phys.*, 2003, **5**, 2842.

(2) P. Vayssière, A. Chaumont and G. Wipff, *Phys. Chem. Chem. Phys.*, 2004, **7**, 124.

(3) A. Chaumont and G. Wipff, *Inorg. Chem.*, 2004, **43**, 5891; *Inorg. Chem.*, 2003, **42**, 5348; *Phys. Chem. Chem. Phys.*, 2003, **5**, 3481; *J. Phys. Chem A*, 2004, **108**, 3311; *Chem. Eur. J.*, 2004, **10**, 3919.