ID de Contribution: **185** Type: **Contribution orale**

Semiclassical modeling of an elementary chemical reaction inside helium nanodroplets

vendredi 7 juillet 2023 09:50 (20 minutes)

Experimental evidence for long-range electron transfer in alkali clusters interacting with fullerene-doped helium nanodroplets was reported by the Scheier group. Such reactions are hindered by the very different propensities of the two reaction partners towards solubility, alkalis being heliophobic while fullerenes are heliophilic.

In this contribution, we present a preliminary investigation of a similar chemical situation, namely the formation of the ionic bond in NaCl from the two initially distant neutral partners, by means of semiclassical computational modeling. Our approach relies on ring-polymer molecular dynamics simulations, that take into account vibrational delocalization but ignore the superfluid character. A reactive potential energy surface is designed from empirical valence-bond theory, both neutral and ionic states being dressed by the helium solvent with appropriate polarization forces for the ionic state.

Two conditions were considered for triggering the reaction, either through an adiabatic collision between one isolated parner and the solvated, other partner, or the progressive shrinking of the droplet by solvent evaporation. In both cases, nuclear delocalization is found to influence not only the solvent itself, but also the NaCl solute upon its formation.

Affiliation de l'auteur principal

Laboratoire Interdisciplinaire de Physique

Auteur principal: CALVO, Florent (CNRS)

Orateur: CALVO, Florent (CNRS)

Classification de Session: Mini-colloques: MC05 Physico-chimie des environnements atomiques et moléculaires froids et ultra froids

Classification de thématique: MC5 Physico-chimie des environnements atomiques et moléculaires froids et ultra froids