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ΘΕΜΑ: Fragmentation processes of charged aqueous clusters
Διάσπαση φορτισμένων υδατικών συσσωματωμάτων

ΤΟΠΟΣ: Αίθουσα Σεμιναρίων ΙΤΕ/ΕΙΧΗΜΥΘ

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ΠΕΡΙΛΗΨΗ

Fragmentation processes of mesoscopic aqueous clusters charged with ions of similar sign are studied by computer simulations. The systems contain Na+, Cl− and mixtures of ions embedded in clusters composed of several hundreds of water molecules. The ratio of the number of ions over that of the solvent molecules is such that the clusters are stable for several nanoseconds.

Fragmentation is caused by infrequent shape fluctuations. A new reaction coordinate is introduced that captures the shape changes that determine the reaction mechanism and allows for the study of the fragmentation mechanism using theories of activated processes. The nature of the shape fluctuations responsible for the fragmentation is characterized by free energy profiles computed as function of the new reaction coordinate. Dynamics of the fragmentation shows that the barrier crossing is diffusive so that the dynamical corrections to the transition state are large. The structure of the decay of the time-dependent rate constant reflects the diffusive character of the recrossing dynamics so that a plateau is established after a long transient time of 5 ps. The free energy and dynamics of the reaction demonstrate that clusters fragment unevenly in contrast to predictions of analytical theories.