RUHR-UNIVERSITÄT BOCHUM

RESOLV
RUHR EXPLORES SOLVATION
CLUSTER OF EXCELLENCE - EXC 1069

RUB

# RESOLV: VORTRAGSANKÜNDIGUNG

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# "Cooperative slowdown of water rotation by single pairs of densely charged ions"


Abstract: We use classical atomistic molecular dynamics simulations and polarizable models to investigate the dynamics of rotation of water in the vicinity of single ion-pairs of magnesium sulfate or cesium chloride ions at varying anion-cation separation. Water rotation is markedly slowed down in the first and second hydration layers of the isolated magnesium ion and in the first hydration layer of isolated sulfate and chloride ions; in contrast, isolated cesium ions have almost no effect on water rotational dynamics. At 12 Å anion-cation separation, a small population of water molecules halfway between the magnesium and sulfate ions rotates more slowly than the equivalent population near the isolated ions or near the cesium chloride pair. This result indicates that pairs of densely charged anions and cations weakly slow down water rotation in a cooperative manner even at this large anion-cation separation. Surprisingly, this subpopulation consists exclusively of water molecules in the second or third hydration layers of either ion. In contrast, for a 5 Å anion-cation separation, intense cooperative slowdown of water rotation is observed in the first hydration layer of all four ions, and weak cooperative slowdown is present in the outer hydration layers. Our results broadly support the existence of both short- and long-range cooperative slowdown of water rotation by ions but suggest that intense cooperative slowdown is limited to the first hydration layers of the ions. The dependence of cooperative slowdown on the identity of the ions, anion-cation distance and the position of water molecules relative to the ions obtained from simulations can be used to refine the interpretation of experimental measurements to gain further insight into these systems.


Alle Interessenten sind zur Teilnahme am Vortrag herzlich eingeladen.