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TITLE: Initial stages of salt dissolution: Ion or ion pair solvation?

ABSTRACT:

The interaction of water with rock salt (NaCl) is important in a wide variety of natural processes and human activities. Although NaCl dissolution is a well known process on the macroscale, a detailed atomic scale picture is still missing. Here we report an extensive series of density functional theory, forcefield and molecular dynamics studies of water clusters at flat and defective NaCl surfaces. By comparing structures and energies of different water clusters we try to answer seemingly elementary questions such as how many water molecules are needed before it becomes favourable to extract an ion or ion pair from the crystal.

It turns out, however, that the answers to these questions are not so straightforward: solvation of a single ion is less costly for small water clusters whereas for larger clusters (above 12 molecules) solvation of ion pairs is favoured.