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The initial stages of NaCl dissolution: Ion or ion pair solvation?

JIRI KLIMES, ANGELOS MICHAELIDES, London Centre for Nanotechnology and Department of Chemistry, University College London — The interaction of water with rock salt (NaCl) is important in a wide variety of natural processes and human activities. A lot is known about NaCl dissolution at the macroscopic level but we do not yet have a detailed atomic scale picture of how salt crystals dissolve. Here we report an extensive series of density functional theory, forcefield and molecular dynamics studies of water clusters at flat and defective NaCl surfaces and NaCl clusters. The focus is on answering seemingly elementary questions such as how many water molecules are needed before it becomes favorable to extract an ion or a pair of ions from the crystal or the cluster. It turns out, however, that the answers to these questions are not so straightforward: below a certain number of water molecules ($\sim$ 12) solvation of individual ions is less costly and above this number solvation of ion pairs is favored. These results reveal a hitherto unknown complexity in the NaCl dissolution process born out of a subtle interplay between water-water and water-ion interactions.

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