Adsorption of small NaCl clusters on surfaces of silicon nanostructures

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We have studied possible adsorption geometries of neutral NaCl clusters on the disordered surface of a large silicon model tip used in non-contact atomic force microscopy. The minima hopping method was used to determine low energy model tip configurations as well as ground state geometries of isolated NaCl clusters. The combined system was treated with density functional theory. Alkali halides have proven to be strong structure seekers and tend to form highly stable ground state configurations whenever possible. The favored adsorption geometry for four Na and four Cl atoms was found to be an adsorption of four NaCl dimers due to the formation of Cl-Si bonds. However, for larger NaCl clusters, the increasing energy required to dissociate the cluster into NaCl dimers suggests that adsorption of whole clusters in their isolated ground state configuration is preferred.

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