

Abstract Submitted
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Textbook adsorption at non-textbook adsorption sites: alkali atoms on alkali halide surfaces BO LI, ANGELOS MICHAELIDES, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft — Density-functional theory (DFT) and second order Møller-Plesset perturbation theory (MP2) calculations for F, Cl and Br adatoms on the (100) surfaces of NaF, NaCl and NaBr indicate that on these surfaces the halide adatoms adsorb preferentially above halide substrate sites, rather than above Na substrate sites as might be anticipated. Analysis of the electronic structures in each system reveals that this hitherto unheard of adsorption mode is stabilized by the formation of perfectly conventional covalent bonds between the halide adatoms and the halide substrate atoms. This finding has implications to, for example, alkali-halide crystal growth, atomic manipulation on insulator surfaces, and the design of accurate empirical potentials to describe insulator-adatom interactions.

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