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Electron-Stimulated Emission of Na Atoms from NaCl Nanocubes DAVIDE CERESOLI, TANYA ZYKOVA-TIMAN, SISSA, Trieste, ERIO TOSATTI, SISSA and ICTP, Trieste — Emission of neutral cations/anions from solid akali halides can in principle be provoked by donating/subtracting electrons to the surface of alkali halide crystals, but generally constitutes a very endoenergetic process. The amount of energy required is expected to decrease for atoms located in less favorable positions, such as at surface steps and kinks, where the local coordination is smaller. The most favorable case of all should be represented by corner atoms of alkali halides cubes, where ionic binding is the weakest. We carried out first principles density functional calculations and simulations of magic-size neutral and charged NaCl nanocubes, to ascertain the stability and extractibility of neutralized corner ions. We find that detachment of neutral Na atoms upon donation of an excess electron is possible for a very modest energetic cost of the order of 0.6 eV, in line with early experimental observations. The atomic and electronic structure of the resulting Na^+ vacancy is analyzed in detail.

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