Prediction of formation of layered ultrathin graphene-type films of ionic compound

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Abstract Structural changes at surfaces including atomic relaxation and reconstruction are a manifestation of their effort to minimize the total free energy. Atomic rearrangements are typically moderate at surfaces of semi-infinite systems and in thick slabs in order to minimize the energy penalty associated with structural mismatch at the interface between the reconstructed surface and the unreconstructed bulk. In ultra-thin slabs, surface contribution dominates the total energy, as only a small fraction of atoms experience bulk-like atomic environment.

Our results based on ab initio density functional calculations indicate a general graphitization tendency in ultrathin slabs of ionic compound including rocksalt and cesium chloride-type structures. Whereas the bulk of many compounds show an energy preference for cubic rather than layered atomic arrangements, the surface energy of layered systems is commonly lower than that of their cubic counterparts. We determine the critical slab thickness for range of systems, below which spontaneous conversion from cubic to layered graphitic structure occurs, driven by surface energy reduction in surface-dominated structures. Such graphitization process was investigated in details for cubic sodium chloride thin slabs.

Figures