Supporting Information for:

Spontaneous graphitization of ultrathin cubic structures: A computational study

Pavel B. Sorokin, Alexander G. Kvashnin, Zhen Zhu, and David Tománek
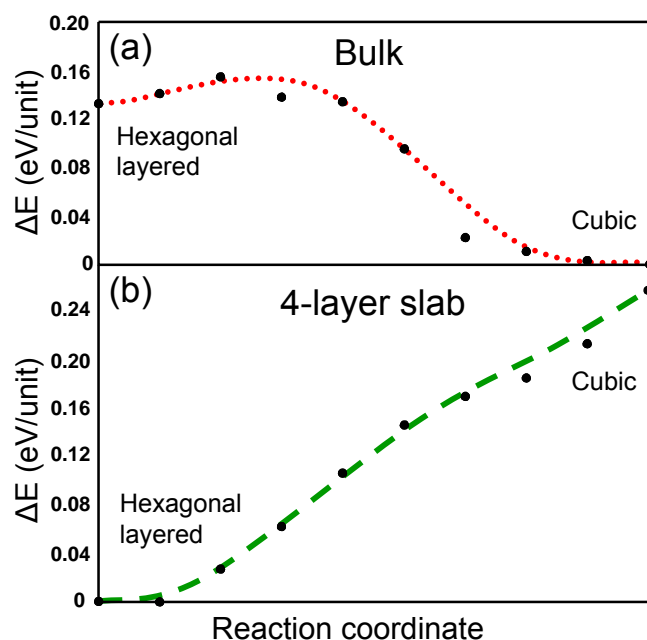

FIG. S1. (Color online) Energetics of the cubic-to-hexagonal transition (a) in bulk and (b) in a 4-layer slab of NaCl with (111) surfaces. The reaction coordinate characterizes the geometries encountered during the transition. Energies are given per stoichiometric unit. The lines are guides to the eye.

ENERGETICS OF THE CUBIC-TO-HEXAGONAL TRANSITION IN NACL

We present the energy encountered by NaCl during a cubic-to-hexagonal transition in Fig. S1. Figure S1(a)

represents the bulk and Fig. S1(b) an ultra-thin (4-layer) slab. The reaction coordinate covers likely transition geometries ranging from the "layered hexagonal" structure on the left to the "cubic" structure on the right.

Even though the cubic phase is most stable for bulk NaCl, the layered hexagonal phase appears as a metastable state. As seen in Fig. S1(a), the metastable state is protected by a low activation barrier from transforming to the cubic phase.

The situation is very different in ultra-thin NaCl slabs. As seen in Fig. S1(b), the layered hexagonal structure is most stable in this case. Even more interesting is the fact that a structural transformation from the cubic to the layered hexagonal phase does not involve an activation barrier.

The relative stability of the cubic and layered hexagonal phase is presented as a function of the number of layers in Fig. 2 of the main manuscript. In few-layer systems, where the layered hexagonal phase is energetically preferred, we find the structural transition to generally involve an activation barrier that decreases and eventually vanishes with decreasing slab thickness.

A picture similar to NaCl emerges also for ultra-thin slabs of other substances with a stable bulk cubic phase.