Graphene, borophene, and… ceramics—theory sampling, from interesting to important

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In research, an interesting intellectually compelling problem and even its elegant solution do not always lead to practical impact. In reversal, challenging, important practical problems are rarely easily articulated as scientific questions, before good answers can be even contemplated. Our examples involve carbon, boron, and ceramics materials, all of interest to this forum. Producing large area graphene, continuously and as single crystal, with no grain boundaries, has been of great interest, in order to scale up its electronics feasibility. We will sketch one approach relying on kinetic differentiation and competition of misoriented domains in "evolutionary selection" growth, and show how it ultimately can yield an unlimited, in principle, sp^2-carbon network of single crystal coherence [I. Vlassiouk, BIY, et al., Nature Mater. 17, 318, 2018].

Borophene, a two-dimensional boron, has sprung to the research arena following our prediction of the boron fullerene B_{80}. All 2D-planar borophene phases are metals, although depend on the substrate electron donation. Recent studies demonstrate hard bilayer borophene with promising superconductivity (predicted T_c = 25-45 K), and low work function. Will this fascinating material, already synthesized, remain in the realm of scientific quest, rewarding yet ultimately academic, or it may eventually impact our daily life---on this question, the jury is still out.

On the other side of the spectrum of *important* are ceramics, born in the heat of kilns, not academic debates, and a challenge to unravel molecular mechanisms of synthesis and sintering. It came to the fore with demand for UHTC, ultra-high temperature ceramics for aerospace and supersonics shields. I will share experience in developing theory of so-called flash synthesis, accelerated by a Joule-heat spike. Focusing on an iconic YSZ, yttria-stabilized zirconia, we argue that there is a feedback-loop involving thermal sublimation of mobile O-sublattice, creating the vacancies V_O^{2+} (e-donors), to shift the Fermi level above the charge-transition levels, CTL ($E_F > E_{CTL}$). This triggers the charge-state change of the Zr-vacancies, $V_{Zr}^{0} \rightarrow V_{Zr}^{-4}$, reducing its hopping barrier, and giving it higher diffusivity, thus accelerating the sintering.