Boundary Effects on the Electronic States of Nanomaterials

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In this talk, I will show that boundary has profound effects on the band gap of a perfectly passivated nanostructure. Taking, for example, hydrogenated zigzag graphene nanoribbon where the lowest-energy edge has a period of three. As such there exist two edge polymophs. The two are related to each other by sliding one of the two edges by one third of the lattice parameter. This simple operation to ribbons of identical size and shape can result in distinctly different electronic structures but identical formation energy. In particular, the band gaps can differ by more than a factor of two. In other words, a graphene nanoribbon may not have a well-defined band gap. The boundary effects may also exist in other semiconductor nanostructures. Taking thin silicon films as an example, I will show that their band gaps depend critically on the pattern of passivation as well as on the chemical identity of the passivating agents, i.e., oxygen or hydrogen. Most strikingly, oxygen passivation can completely eliminate the quantum size effect from the uppermost valence band state. This enables bulklike nanostructures at a size as small as one nanometer, which could be highly desirable for IC applications. A seventeen-year old “trancated crystal” theory [Zhang, Yeh, and Zunger, Phys. Rev. B 48, 11204 (1993)] may provide an explanation to all these seemingly unrelated observations.