Geometries, Electronic Properties, and Materials Design of Carbon Nanostructures and Related Materials

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Ever since the macroscopic production and the experimental confirmation of its presence and stability of C_{60} clusters ("fullerenes") in 1990, carbon nanostructures and related materials have been of high interest and of extreme importance in many fields of science and technology. Fullerenes are zero-dimensional sp^2 carbon materials, while carbon nanotubes and graphene are one- and two-dimensional sp^2 carbon materials, respectively. Due to the locally resilient nature of C-C bonds and to the globally flexible nature of the sp^2 network, one can consider in principle an infinite number of different carbon nanostructures. More importantly, many carbon nanostructures theorists had considered or designed have actually been produced or found experimentally so far. The importance of the collaborative research by theorists and experimentalists in this research field and the consequent progress will become even greater in the future since the variation of the nanostructured materials is increasing.

In this talk first I will introduce our several previous attempts to design mixeddimensionality carbon nanostructured materials using graphene [1-3], and next I will show the graphene-based new functional materials which we designed and are yet to be produced experimentally [4]. Also the proposal of the periodical geometry modification of graphene [5] and its recent progress will be reviewed [6]. Finally, I will show our recent results on the composite materials of graphene and the hexiagonal boron-nitride atomic layers [7-9]. I will show the chemically rather strong nature of the interlayer interaction between B and C atoms, which can give rise to the commensurate superlattices and thin films consisting of these two kinds of atomic layers. How the electronic transport properties can be modified by just changing the stacking sequence will be shown as well.

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