Center for Computational Sciences, University of Tsukuba
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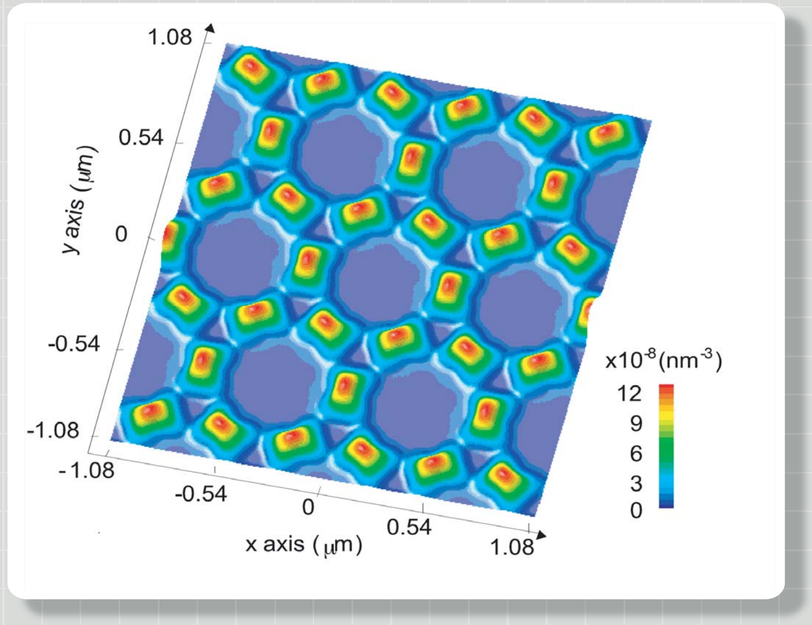
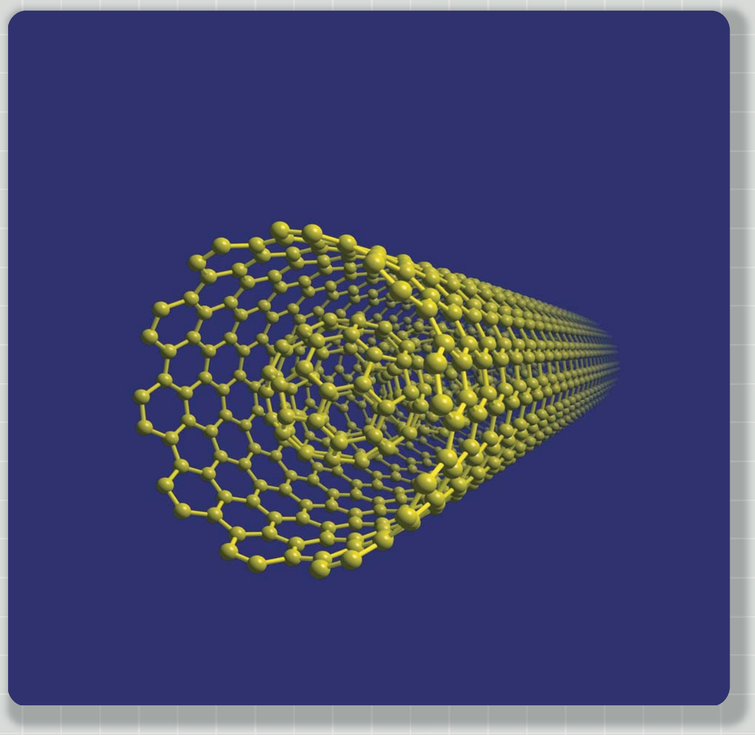
Computational Material and Life Sciences

Design of artificial magnet based on semiconductor quantum wire networks

Physical properties and functions of nanostructures can be substantially controlled by their shapes as well as their constituent elements. We have succeeded to design the artificial ferromagnet fabricated only by non-magnetic InAs semiconductor quantum wires. Moreover, we have found that our designed ferromagnetism can easily be controlled by only applying electric and magnetic field.



Electronic properties of Nano-Carbon Materials



Recently, an interesting complex consisting of fullerenes and nanotubes is synthesized. The material consists of a 1D array of fullerenes which are encapsulated by a carbon nanotube (occasionally called ``peapod"). Our first-principle calculations reveals that the space between the nanotube and the encapsulated fullerenes is a decisive factor to determine the energetics for the encapsulation process of the fullerenes in the nanotubes and the stability of resultant structures. It is also clarified that the electronic structures of peapods depend on the space and that they reflect electron states of the encapsulated fullerenes.

Mechanisms of Self-Cleavage of Ribozymes

RNA that is responsible for transfer of genetic information occasionally works as an enzyme (ribozyme). [The right is a reaction scheme of the self-cleavage of a ribozyme.]. Clarification of the ribozyme function is important in both science and medical application: The ribozyme is a possible tool for gene therapy. Our group has performed the first-principle quantum-theoretical molecular-dynamics calculations for the ribozyme or the first time and identified the reaction athways and obtained the corresponding ree-energy barriers.