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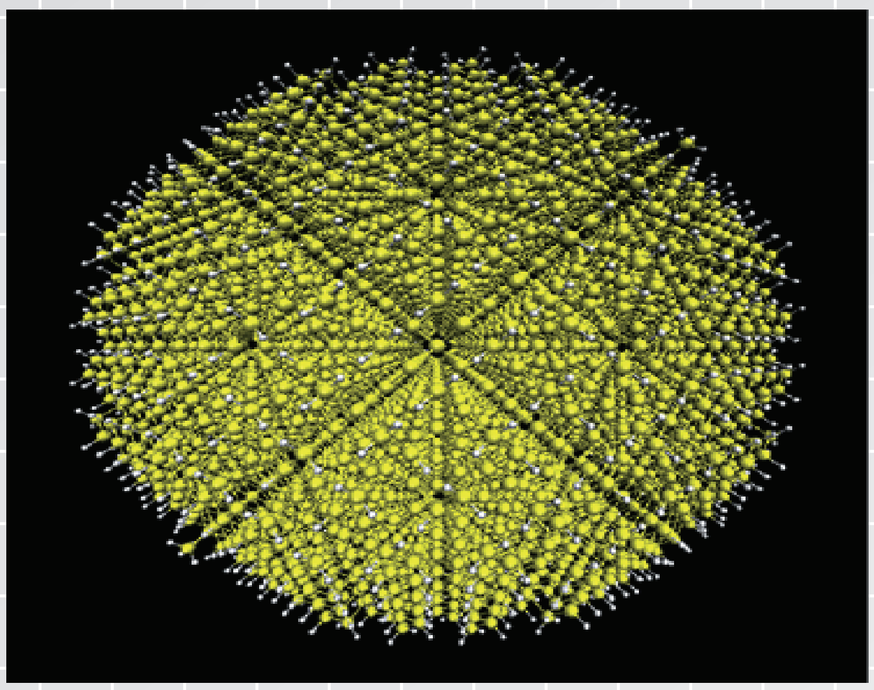
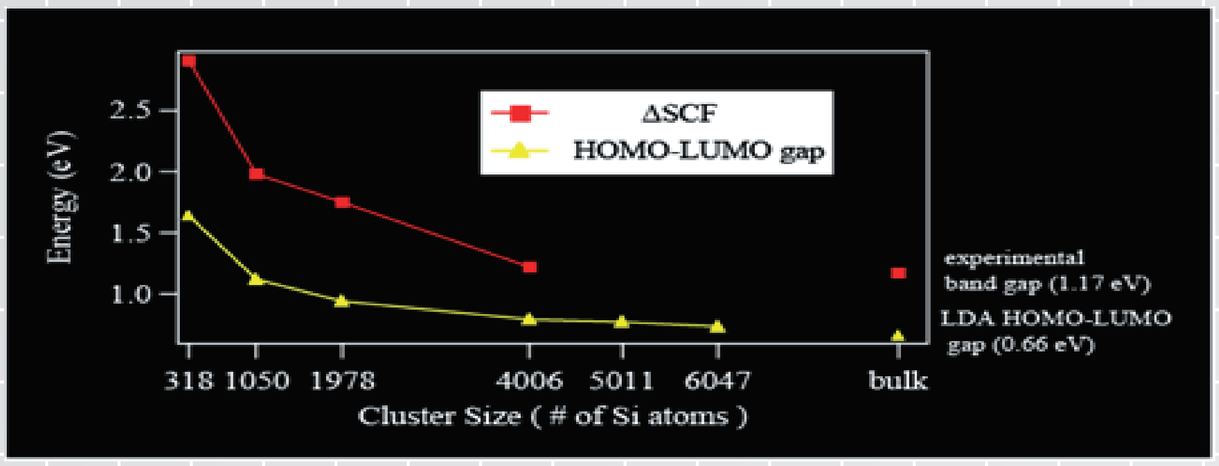
Materials Sciences on PACS-CS

Real-space density-functional theory

We have developed a new scheme of quantum theoretical atomistic simulations based on the Density Functional Theory (DFT). In the scheme, all the calculations are done on lattices in real space (RSDFT). As a consequence, the scheme is free from communication burden of the Fast Fourier Transform, utilize flexible boundary conditions, and is therefore best fitted to next-generation supercomputers with parallel architecture. The target is a nanostructure consisting of 10,000 atoms where new properties such as magnetism in carbon nanotubes may come up. More fundamentally, we are performing total energy calculations for neutral and charged Si clusters to obtain electron excitation energies. In the past, the excitation energies are estimated





from single-electron HOMO-LUMO gap. However, more legitimate way is to obtain them through total-energy difference of charged and neutral materials (ΔSCF). RSDFT now allows us to perform such ΔSCF calculations. The left figure shows calculated ΔSCF gap of Si clusters with more than 6,000 atoms shown above.

Time-dependent density-functional theory

Experimental observations of magnetism in nanometer carbon materials have stimulated a lot of attentions to carbon allotropes as promising candidates for light and stiff magnetic materials which are expected to be applicable to a wide field of modern technology. Vacancies, edges, and negative Gaussian curvature introduced in the honeycomb networks of sp^2 C atoms have been known to result in the magnetism on sp^2 carbon nanomaterials.

Here we design a new magnetic carbon nanotube with topological line defect consisting of pentagon and octagon rings by performing the first-principles total-energy electronic-structure calculations in the density functional theory (DFT). Our DFT calculation certainly show that the nanotube with the topological line defect exhibits magnetic ordering that polarized electron spins are localized around the defect and ferromagnetically aligned along the tube axis. The calculated magnetic moment is about 0.04 μ_B/Å irrespective of the tube diameter studied here. We have analytically shown that the magnetic ordering is induced by the flat band state whose characteristics is the same as the edge states of the graphite ribbons. The nanotubes with the topological line defect are found to be thermally stable and are expected to be synthesized by implanting C_2 clusters in nanotubes or by annealing atomistically defective nanotubes. Our finding is the first evidence of long-range spin ordering expected for the nanotubes of cylindrical shape consisting solely of threefold coordinated sp^2 C atoms.