Mina Maruyama
Susumu Okada

University of Tsukuba, 1-1-1 Tennnodai, Tsukuba, Japan

mmaruyama@comas.frsc.tsukuba.ac.jp

Magnetism and Electronic Polarity of Two-Dimensional Network Consisting of C_{40} Fullerene

Fullerene can form two-dimensional covalent networks by forming interfullerene covalent bonds, being known as fullerene polymers. The electronic structures of fullerene polymers are sensitive to interfullerene bond arrangements, leading to the metallic or semiconducting electronic structures depending on the covalent bonding network topologies [1]. Furthermore, the electronic structures of fullerene polymers also depend on that of the constituent fullerenes. Thus, by assembling the fullerenes with peculiar electronic structures, the resultant polymeric fullerenes are expected to exhibit unusual electronic properties, which are absent in the conventional carbon allotropes. In the present work, we theoretically design the novel two-dimensional C networks comprising small fullerenes with polymeric structures using the density functional theory with the generalized gradient approximation. Among various small fullerenes, we focus on C_{40} with T_d symmetry as a constituent unit of two-dimensional network of polymerized small fullerene, because it possess an acepentalene structure in its cage, which leads to the spin polarization [2].

Figure 1 shows optimized structures of C_{40} polymers with parallel and antiparallel intermolecular arrangements under the optimum lattice constant of 13.5 nm. In polymeric structures, C_{40} is connected to its three adjacent molecules via cycloaddition covalent bonds. Total energies of C_{40} polymers with parallel and antiparallel arrangements are 0.596 and 0.597 eV/atom with respect to that of graphene. Although C_{40} polymers with parallel and antiparallel arrangements are semiconductors with direct band gap of 0.08 and 0.05 eV at M point, respectively, C_{40} polymers possess spin polarization around the apex of molecules as shown in Figure 2, owing to the narrow bandwidth and small band gap. Furthermore, C_{40} polymer sheet possesses electric dipole moment normal to the polymeric layer, owing to their asymmetric molecular shape (Figure 3). In the case of parallel arrangement structure, value of potential difference is changed against the expansion and contraction of lattice constant. Thus, the network is an all carbon two-dimensional material exhibiting both magnetic and electric polarities.

References

[1] S. Okada and A. Oshiyama, Phys. Rev. B, 68 (2003) 235402.
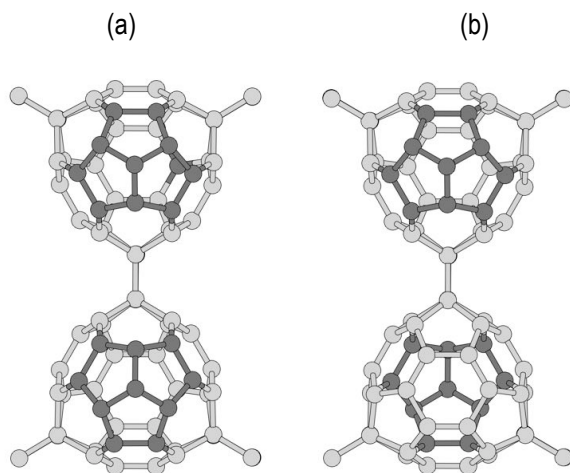[2] M. Maruyama and S. Okada, Appl. Phys. Express, 6 (2013) 095101.

(a)   (b)

Figure 1: Optimized structures of C_{40} polymer with (a) parallel and (b) antiparallel intermolecular arrangements. Black balls denote C atoms belonging to the acepentalene unit in the molecule.
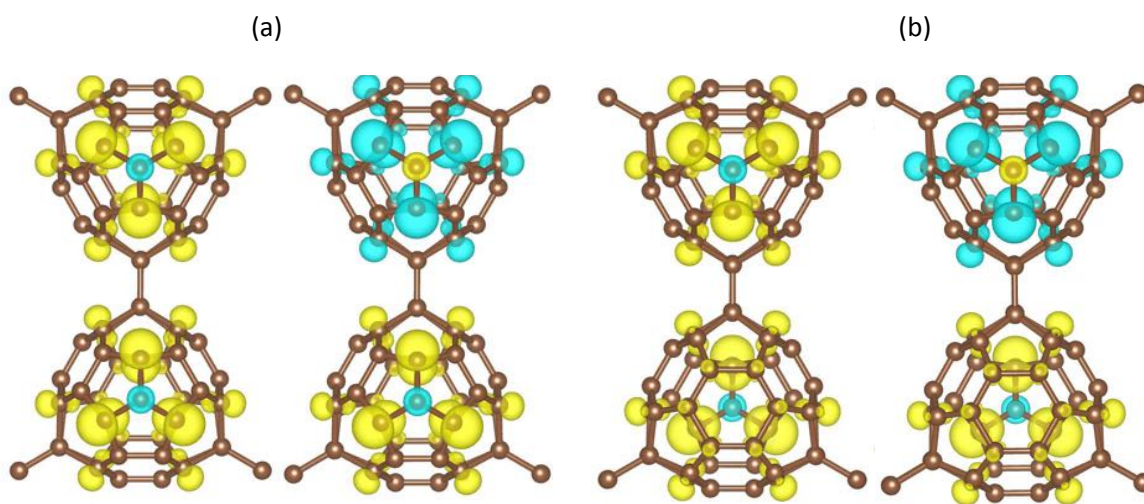
(a)   (b)

Figure 2: Isosurfaces of spin densities of C_{40} polymer with (a) parallel and (b) antiparallel intermolecular arrangements.

(a)   (b)   (c)
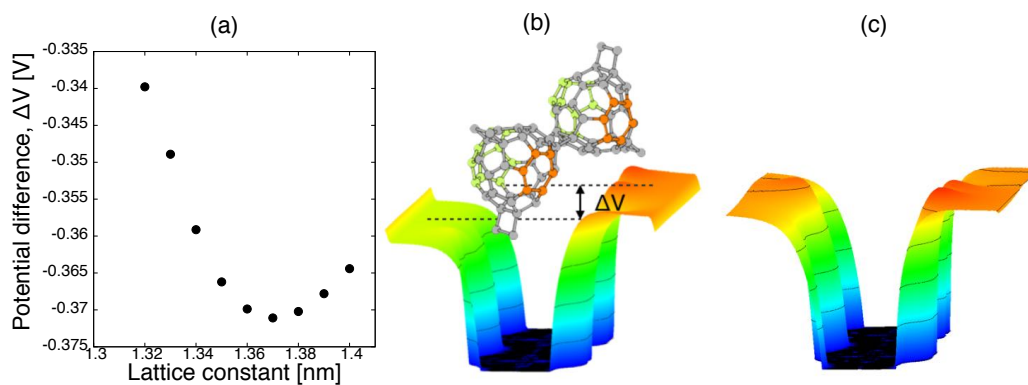

Figure 3: (a) Potential difference normal to C_{40} polymer with parallel arrangement as a function of lattice constant. Contour plots of the electrostatic potential of C_{40} polymer with (b) parallel and (c) antiparallel intermolecular arrangements.