ICCMSE – October 2, 2009

Edge States and Possible Magnetic States in Open-Shell Conjugated Systems

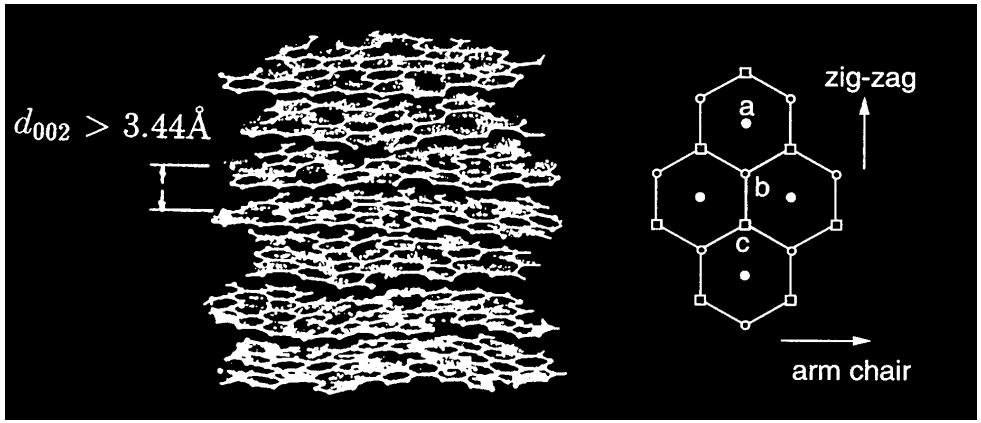
Kikuo Harigaya
Nanotechnology Res. Inst.
AIST, Tsukuba, Japan


Epochal
AIST
my home
土浦市
地図
桜Gセンター
南大通り東
竹園
竹園西小
東新井
千現
ジョモ
倉掛
二の宮公園
物質・材料研究機構
筑波病院
筑波宇宙センター
上広岡
並木小
並木中
小桜南小
並木
並木中等教育学校
二の宮
地質標本館
洞峰公園
産業技術総合研究所
下広岡
二の宮小
松野木
気象研究所
梅園2
大角豆
桜土浦IC
354
55
小東小
谷田部東中
赤塚公園
清掃センター
国立環境研究所
茗渓学園
ココス
稲荷前
アルペン
大角豆
産業技術専門学院
小野川
横山印刷
筑波
常磐道

Outline

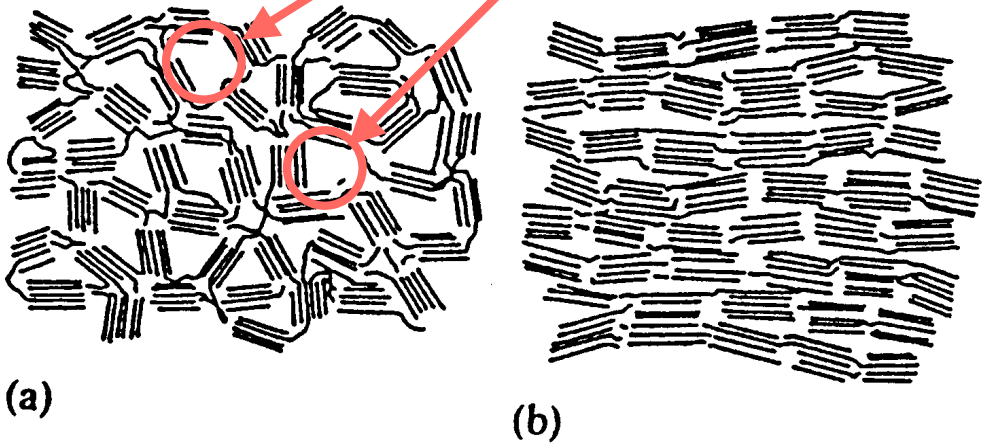
- Possibility of the spin order along the zigzag line of the nanographene was suggested.
- Do the localized spins appear around the lattice defects in fullerene molecules?
- We will consider effects of lattice defect clusters in fullerenes and the bucky bowl molecules.
- The Hubbard model is applied for topological networks of the π-electron lattices.

Stacking of graphene planes

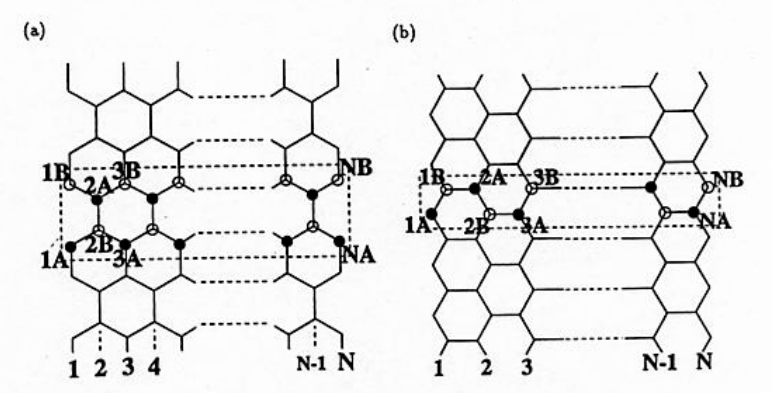


Activated carbon fibers (ACF)

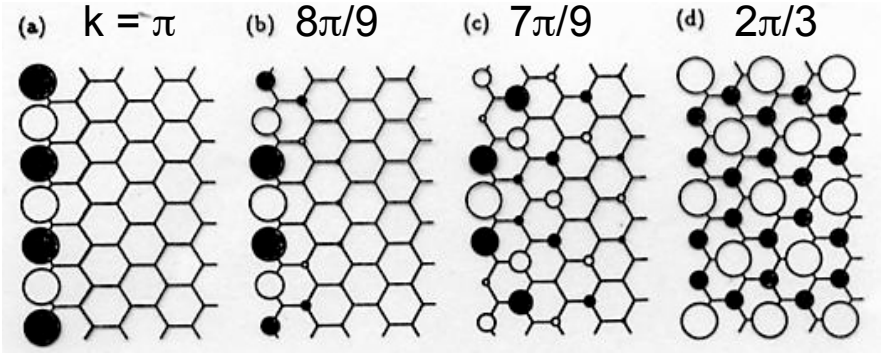
(a) high surface area with nanopore
(structural unites randomly arranged)
(b) a fiber after heat treatment



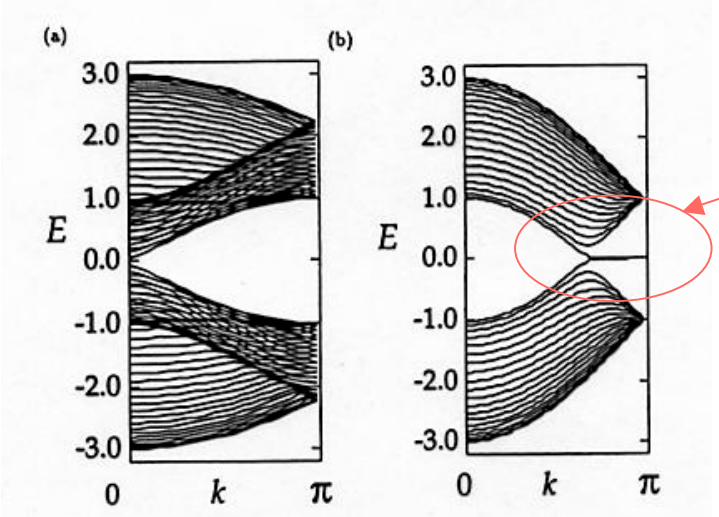
Localized states along zigzag edges



Armchair v.s. zigzag edges



Wave function amplitudes



Band structures of π-electrons

Edge states along zigzag edges

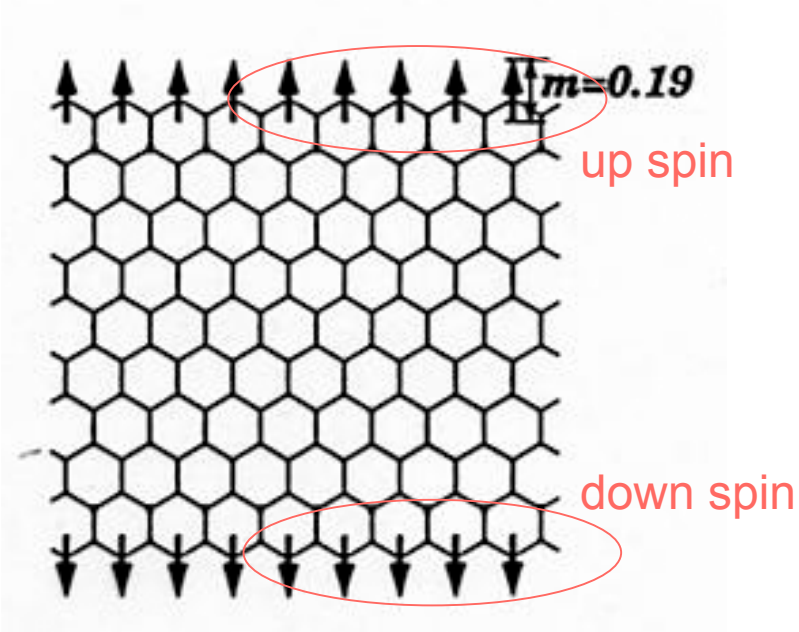
M. Fujita et al, J. Phys. Soc. Jpn. 65 1920 (1996); 66 1864 (1997).

K. Nakada et al, Phys. Rev. B 54 17954 (1996).

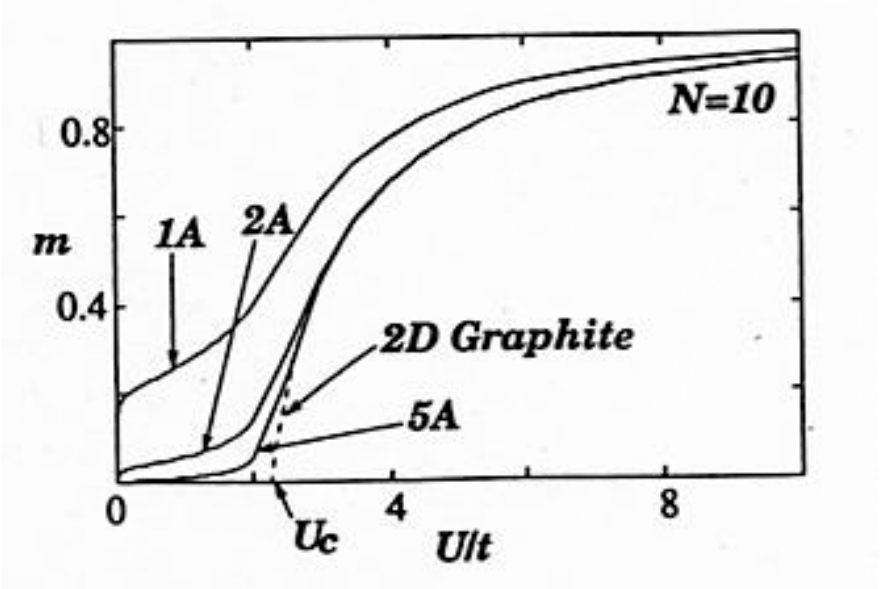
Magnetic moment along the zigzag edge by the Hubbard model

One dimensional Hubbard model for a graphene ribbon

the nearest neighbor hopping t, onsite repulsion U



Spin alignment along the zigzag edges



Spin becomes larger as U increases

Persistence of Edge-State in Stacked Graphene and Nano-Graphene Materials

Kikuo Harigaya*

Nanotechnology Research Institute, AIST, Tsukuba 305-8568, Japan†

(Received)

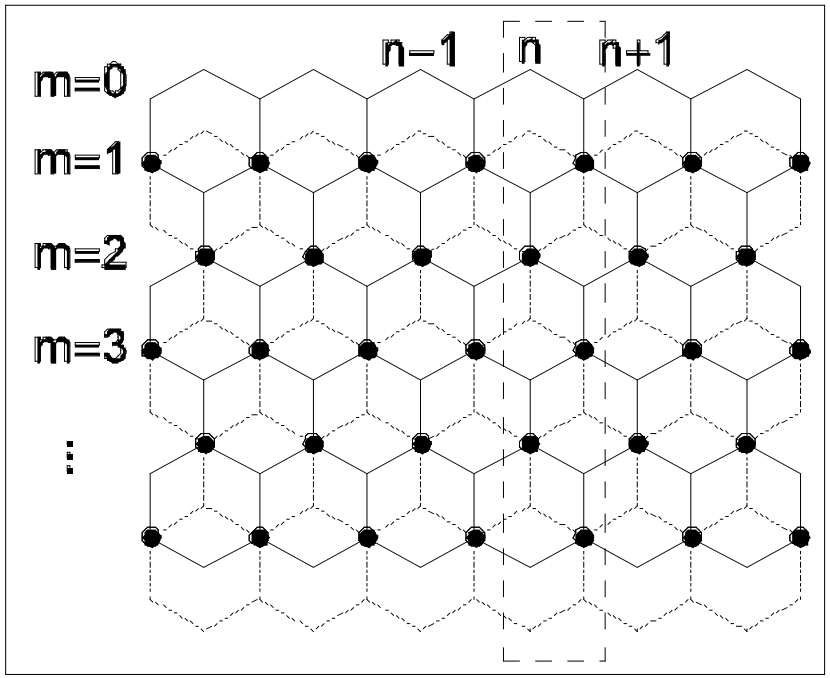
Abstract

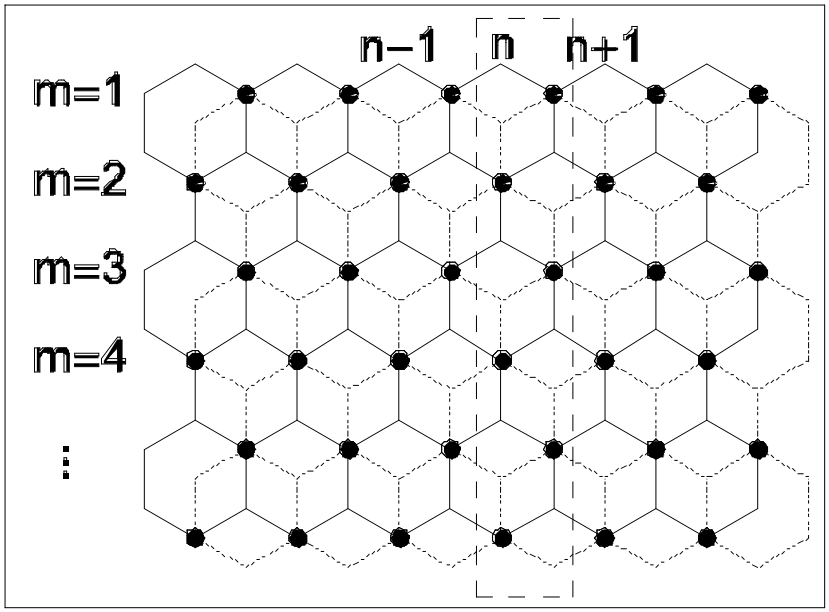
Nano-carbon materials are investigated intensively. In this paper, the edge-state in nanographene materials with zigzag edges is studied theoretically. In particular, while the inter-layer interactions are considered, we prove that edge states exist at the energy of the Dirac point in the doubly stacked nanographene, and in the case of the infinitely-wide lower layer case. This property applies both for the A-B and A-C stackings.

*E-mail address: k.harigaya@aist.go.jp; URL: http://staff.aist.go.jp/k.harigaya/

†Corresponding address

A-B and A-C stackings





upper layer: bold line, lower layer: dashed line,

- interlayer hopping interaction t_1

A-B stacking: upper layer

We will constitute wavefunctions of the edge state. It is assumed that the edge state has amplitudes at the sites of the A sublattice only. The amplitude becomes zero in the B sublattice. Even if the interactions t_1 are present at circles, the alternation of the A and B sites remains in the whole system. So, the bipartite nature remains, too. When we look at the condition of the edge state at the energy $E = 0$ of the upper layer, we find the formula,

$$a_{n,m}\mathrm{e}^{-ika/2} + a_{n+1,m}\mathrm{e}^{ika/2} + a_{n,m+1} = 0, \tag{7}$$

for even m, and

$$a_{n,m}\mathrm{e}^{-ika/2} + a_{n+1,m}\mathrm{e}^{ika/2} + a_{n+1,m+1} = 0 \tag{8}$$

for odd m, where $a_{n,m}$ is the amplitude at the nth unit cell of the mth zigzag line. Assuming $a_{n,0} = A$, we obtain

$$a_{n,m} = A[-2\cos(ka/2)]^m. \tag{9}$$

A-B staking: lower layer

The similar condition of the zero energy state gives,

$$b_{n,m}e^{-ika/2} + b_{n+1,m}e^{ika/2} + b_{n,m+1} + r_1 a_{n,m} = 0 \tag{10}$$

for odd m, and

$$b_{n,m}e^{-ika/2} + b_{n+1,m}e^{ika/2} + b_{n+1,m+1} + r_1 a_{n+1,m} = 0 \tag{11}$$

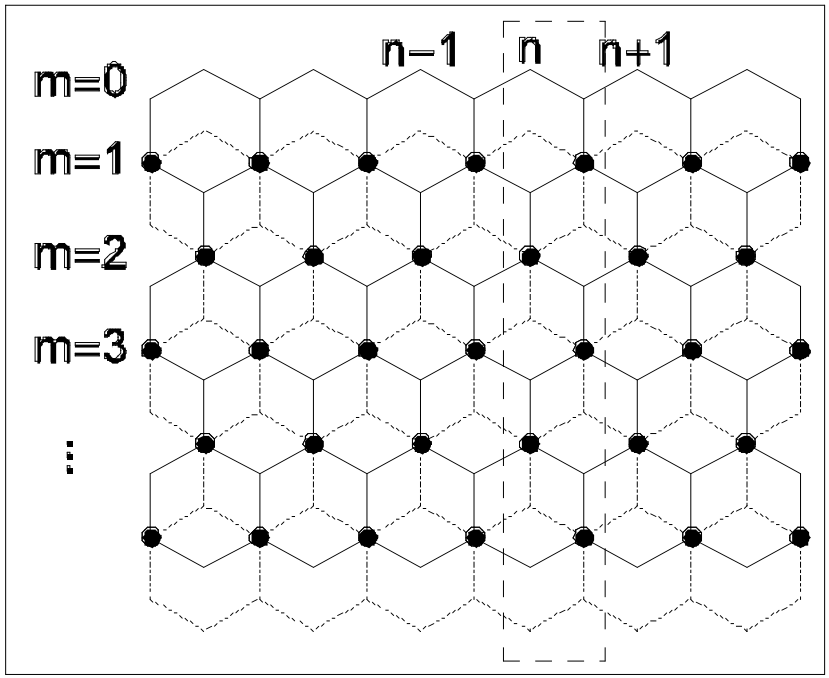
for even m, for the amplitude $b_{n,m}$ of the lower layer. Here, $r_1 = t_1/t$ is the ratio of the interlayer hopping integral to the intralayer hoppings. As we know the form of $a_{n,m}$, we can solve the recurrence formula of the number series to obtain

$$b_{n,m} = -(m-1)r_1 A[-2\cos(ka/2)]^{m-2} + B[-2\cos(ka/2)]^{m-1} \tag{12}$$

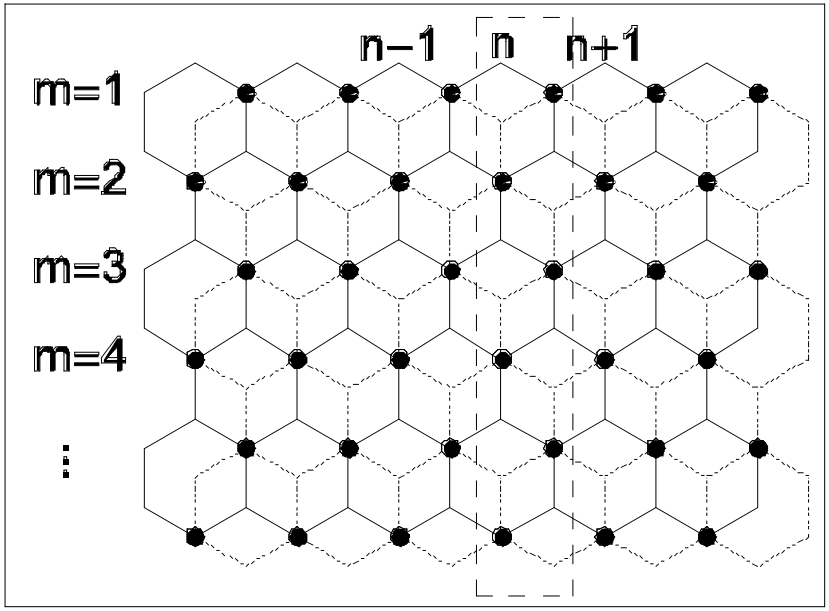
correction of the order $r_1 = t_1/t$

for $m \geq 2$, where $b_{1,m} = B$ is assumed. Therefore, we have found that the edge state persists in the A-B stack case. The magnitudes of A and B will be nearly equal $A \sim B$, so the correction by the interlayer interaction is of the order r_1 with respect to the intralayer term.

A-B and A-C stackings

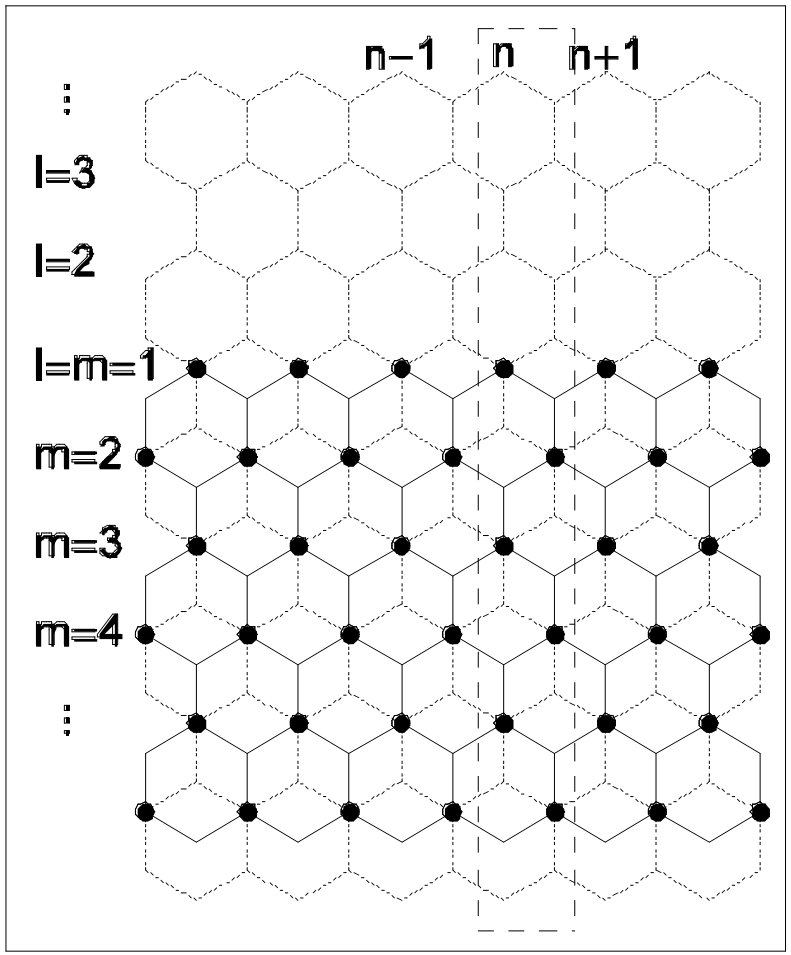


upper layer: no correction by t_1
lower layer: correction present

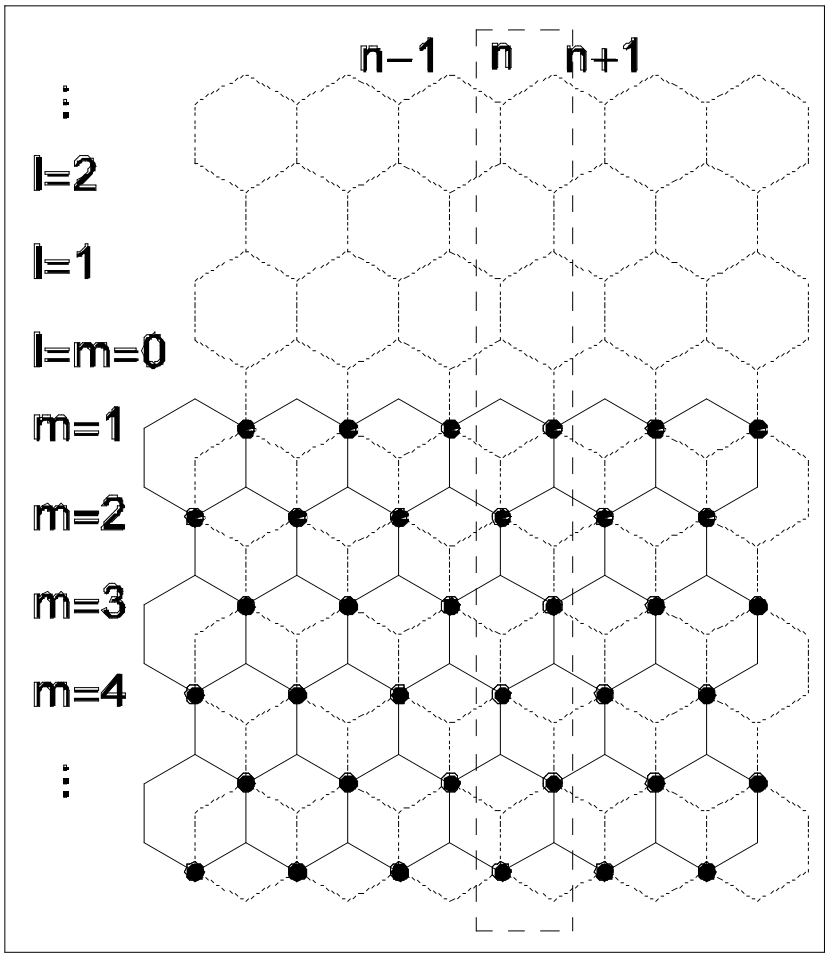


upper layer: correction present
lower layer: no correction by t_1

A-B and A-C stackings



upper layer: no correction by t_1
lower layer: correction present



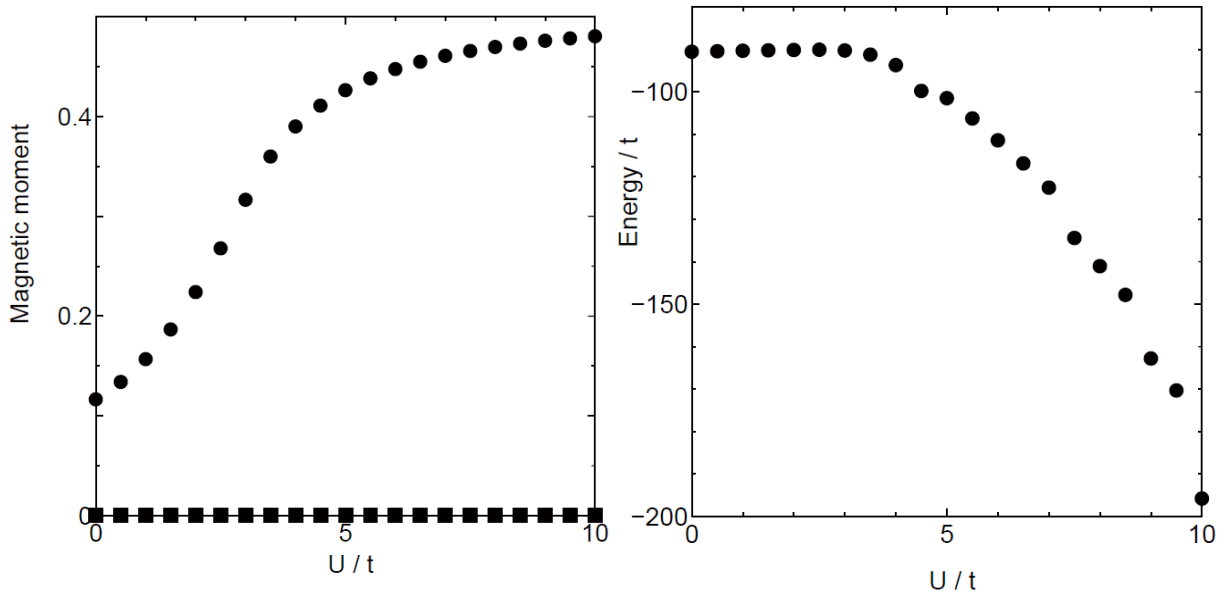
upper layer: correction present
lower layer: no correction by t_1

similarity of the roles in A-B and A-C stackings

Molecule structure of C_{60} and lattice defect clusters

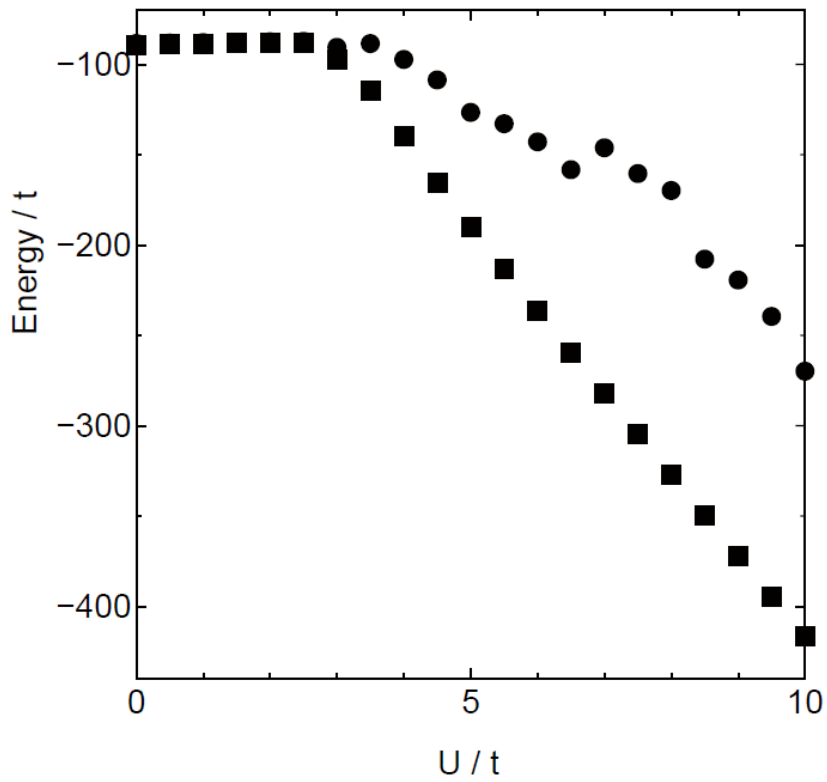
case 1 one defect at the site A
case 2 two defects: A and B
case 3 two defects: A and C
case 4 three defects: A, C, D

case 1



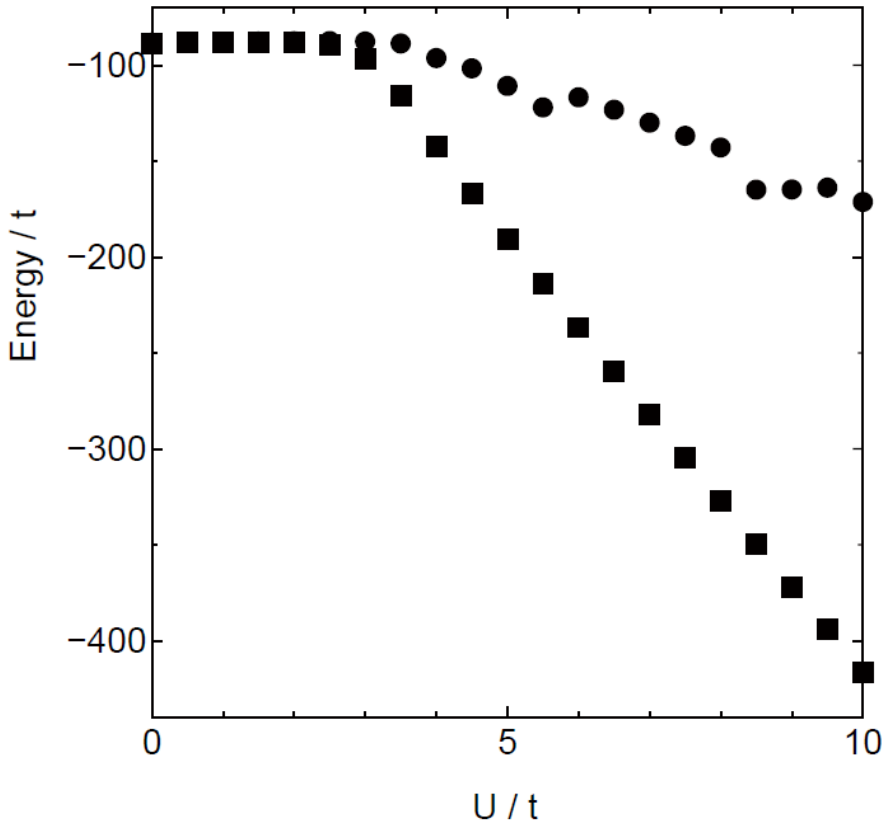
left: magnetic moment: ■ site E, ● site F
right: total energy of the magnetic solution

case 2



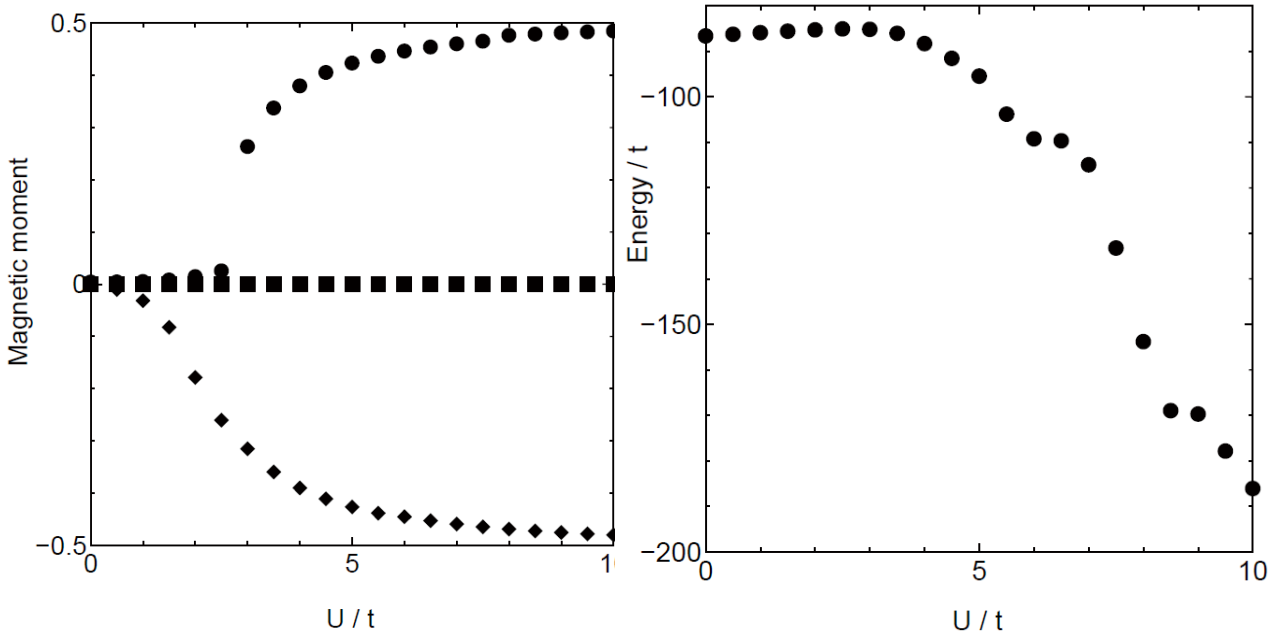
total energy: ● magnetic solution,
■ non-magnetic solution
The non-mag. solution is stable.

case 3



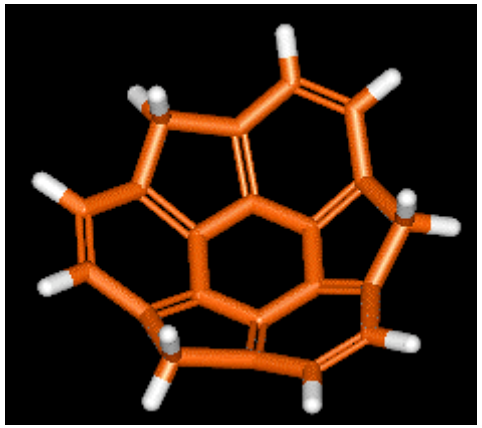
total energy: ● magnetic solution,
■ non-magnetic solution
The non-mag. solution is stable.

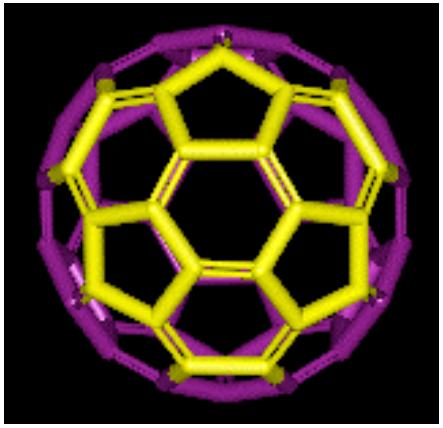
case 4

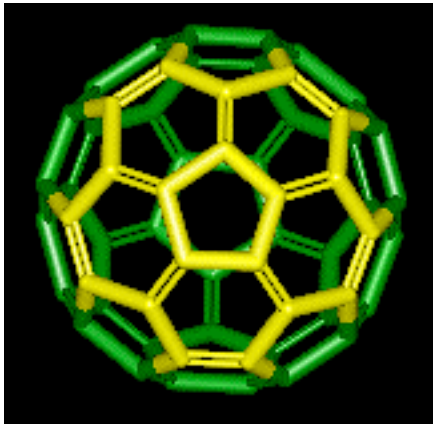


left: magnetic moment: ● site G, ■ site H, ◆ site I
right: total energy of the magnetic solution

bucky bowl - sumanene

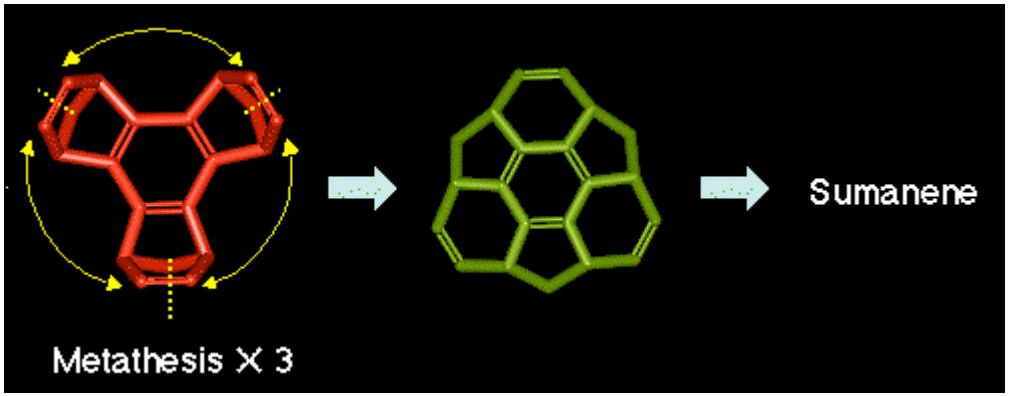




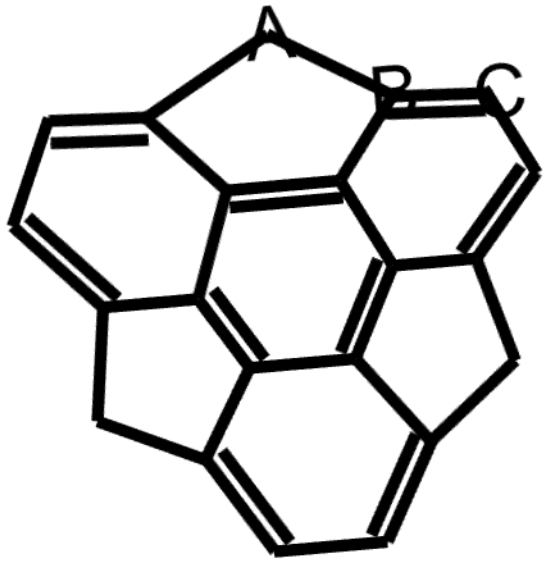


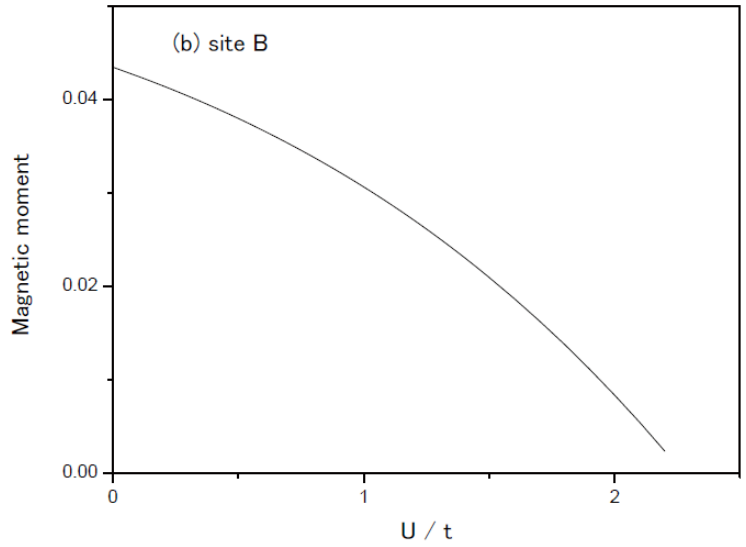
H. Sakurai et al, Science 301, 1878 (2003).
The crystal where the molecules are stacked was obtained.

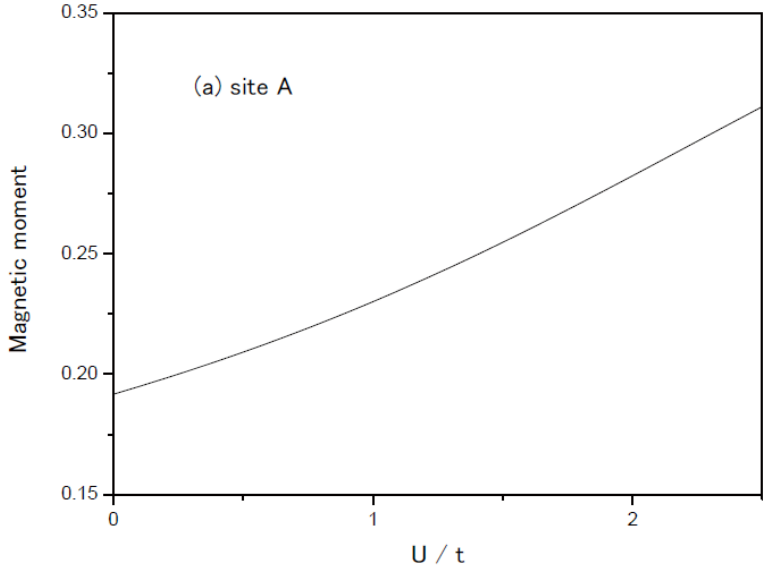
left: sumanene, right: collanulene

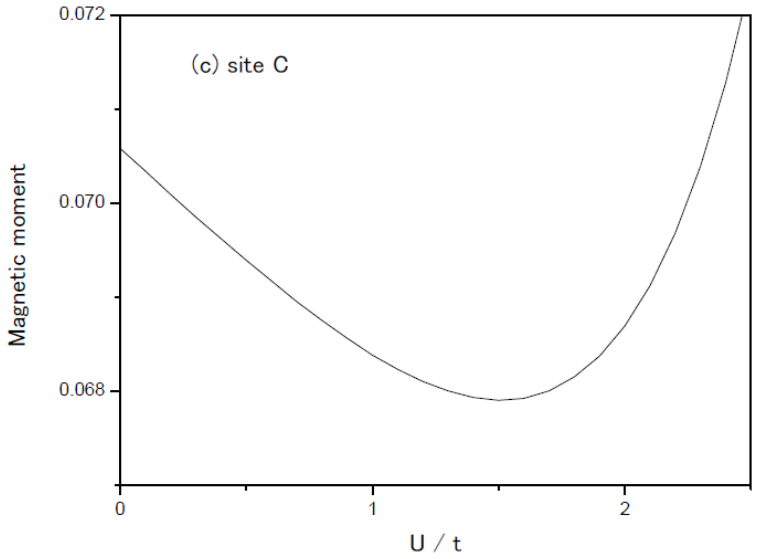


sumanene

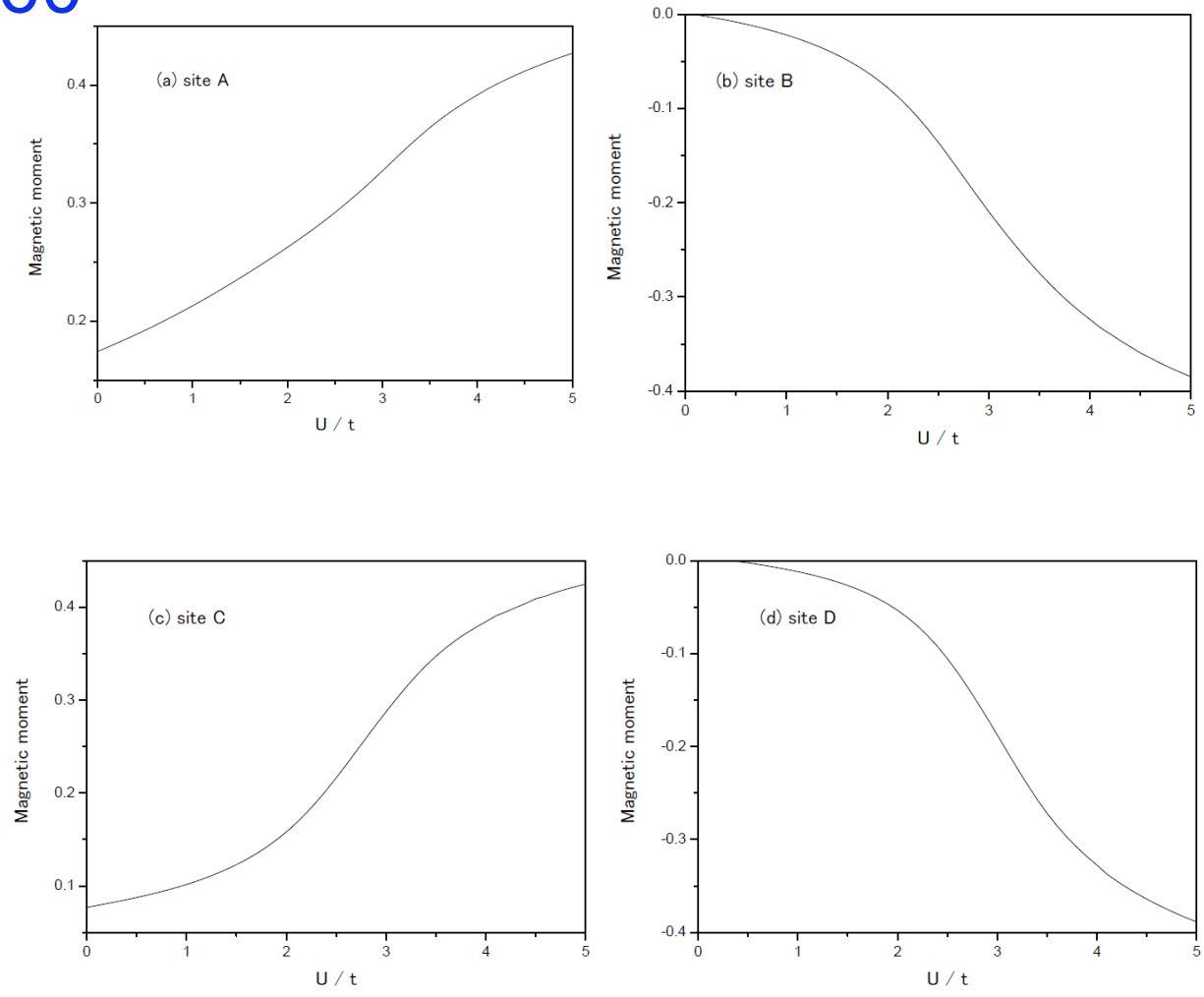

A
B
C


(b) site B
Magnetic moment
0.04
0.02
0.00
0
1
2
U / t


(a) site A
Magnetic moment
0.35
0.30
0.25
0.20
0.15
0
1
2
U / t


(c) site C
Magnetic moment
0.072
0.070
0.068
0
1
2
U / t

a part of C_{60}

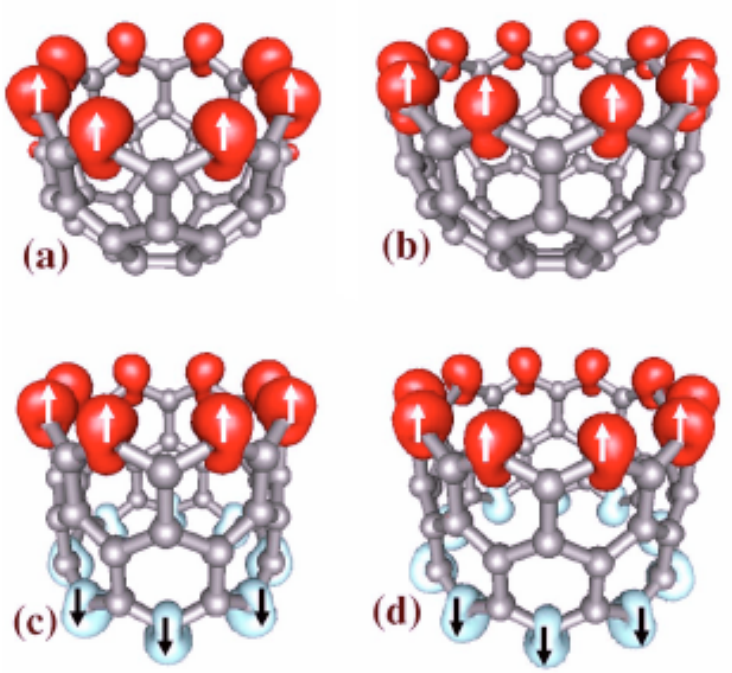


PHYSICAL REVIEW B 68, 125420 (2003)

Defective fullerenes and nanotubes as molecular magnets: An *ab initio* study

Yong-Hyun Kim,* Jin Choi, and K. J. Chang†
Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea

David Tománek‡
Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824-2320, USA
(Received 13 February 2003; revised manuscript received 3 July 2003; published 26 September 2003)



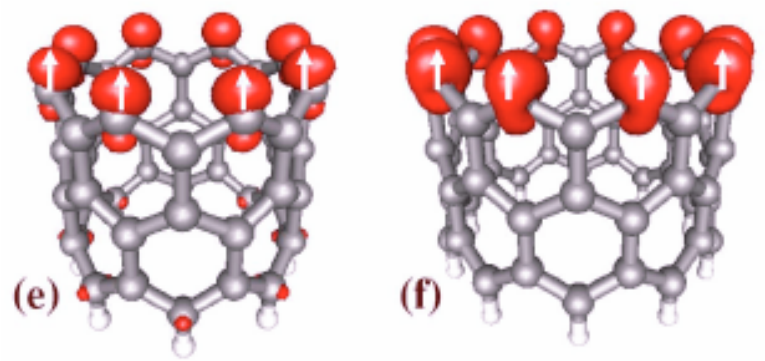


FIG. 3. (Color online) Spin-density isosurfaces for ground-state spin configurations of various (8,0) and (10,0) nanotube segments: dome terminated (a) (8,0) and (b) (10,0) with ferromagnetic ordering; unterminated (c) (8,0) and (d) (10,0) with antiferromagnetic ordering; and hydrogen-passivated (e) (8,0) and (f) (10,0) with ferromagnetic ordering. H atoms are represented by white balls. Red-dark (blue-white) isosurfaces represent equal densities of spin-up (spin-down) electrons, as indicated by arrows.

Summary: contents of this preprint

Persistence of Edge-State in Stacked Graphene and Nano-Graphene Materials

Kikuo Harigaya*

Nanotechnology Research Institute, AIST, Tsukuba 305-8568, Japan†

(Received)

Abstract

Nano-carbon materials are investigated intensively. In this paper, the edge-state in nanographene materials with zigzag edges is studied theoretically. In particular, while the inter-layer interactions are considered, we prove that edge states exist at the energy of the Dirac point in the doubly stacked nanographene, and in the case of the infinitely-wide lower layer case. This property applies both for the A-B and A-C stackings.

Summary

1. When the number of lattice defects is even, magnetic and non-magnetic solutions are obtained. The total energy of the non-mag. solution is lower. Localized spins are suppressed for finite Coulomb interactions.
2. When the defect number is odd, the magnetic solution only appears. The spin alignment appears around the defects, reflecting the symmetries of the molecule.
3. Further, possible magnetism has been analyzed for bucky bowl molecules. The sumanene shows molecular magnetism, while a part of C_{60} shows spin alternation along the zigzag edge of the molecule.