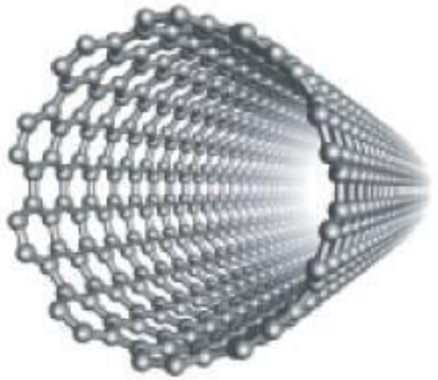
HOMO-LUMO GAPS IN ZIGZAG CARBON NANOTUBES WITH STONE-WALES DEFECT

Noriyuki Mizoguchi

General Education and Research Center, Meiji Pharmaceutical University, 2-522-1, Noshio, Kiyose, Tokyo, Japan

1. Introduction

Carbon nanotubes are not infinite, but finite, and therefore, they always present edges.

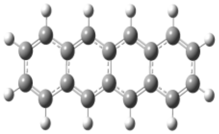


An interesting aspect of finite-length carbon nanotubes (CNTs) is the quantum finite-size effects of the energy gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO).

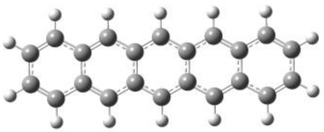
How do the HOMO-LUMO gaps change with the increase of the sizes of the systems ?

In almost cases the HOMO-LUMO gaps of molecules decease monotonically with the increase of the sizes of the systems.

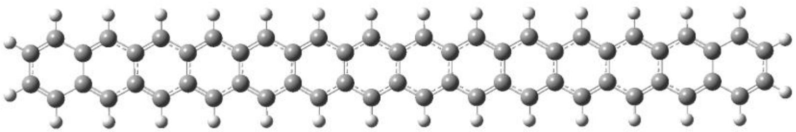
Eample1



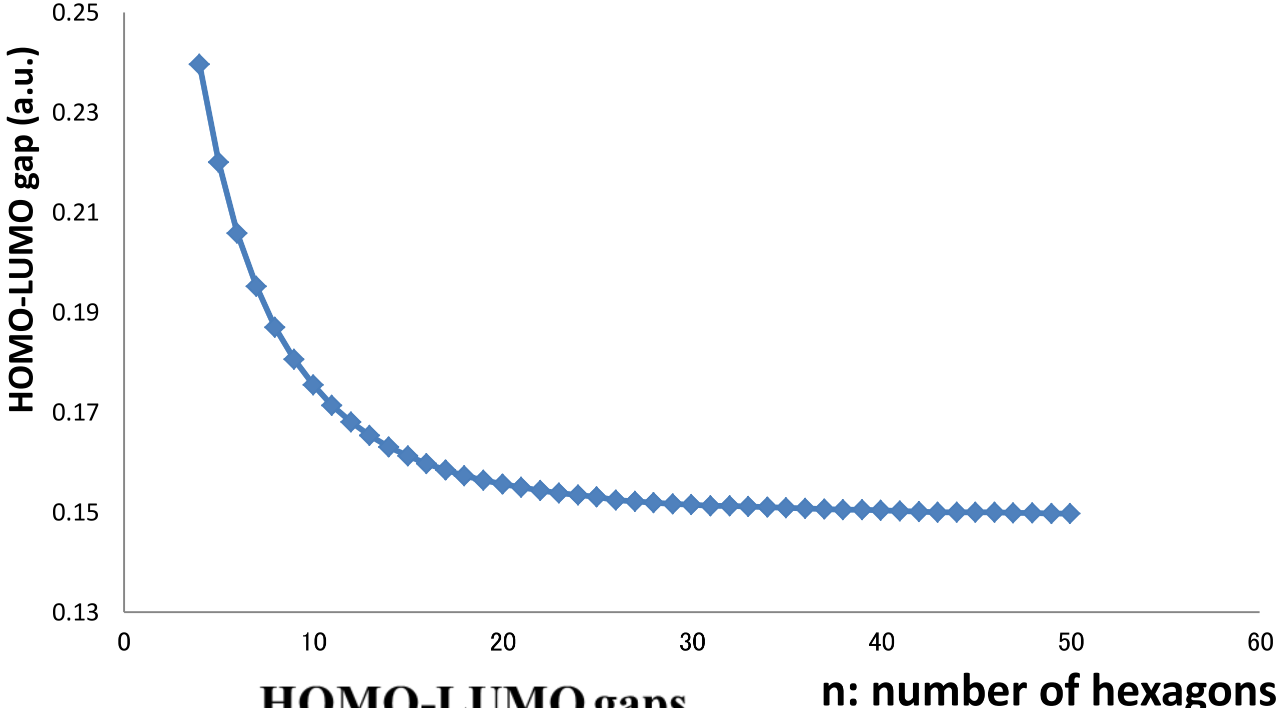
n=4



n=5



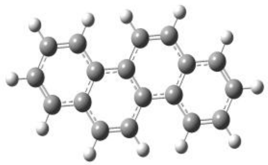
n=14



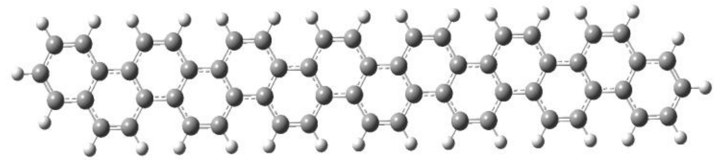
HOMO-LUMO gaps

The HOMO-LUMO gaps of molecules in this series decease monotonically with the increase of the number of hexagons in the systems.

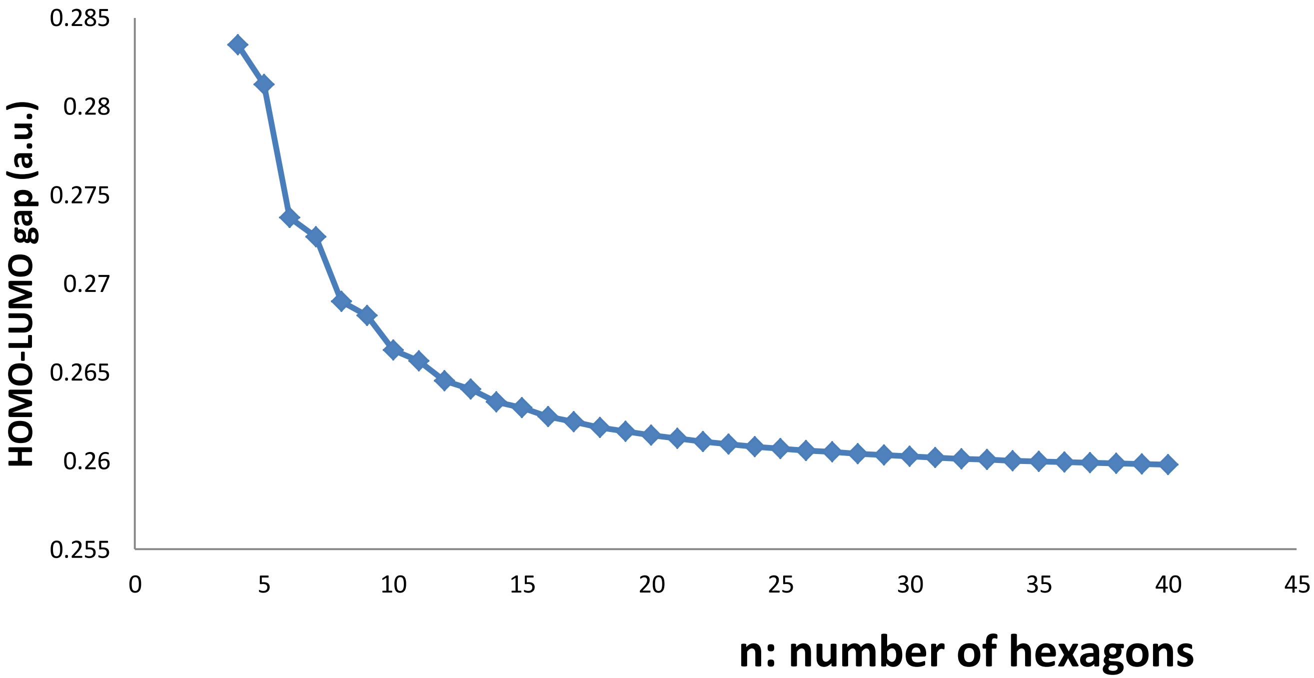
Eample2



n=4



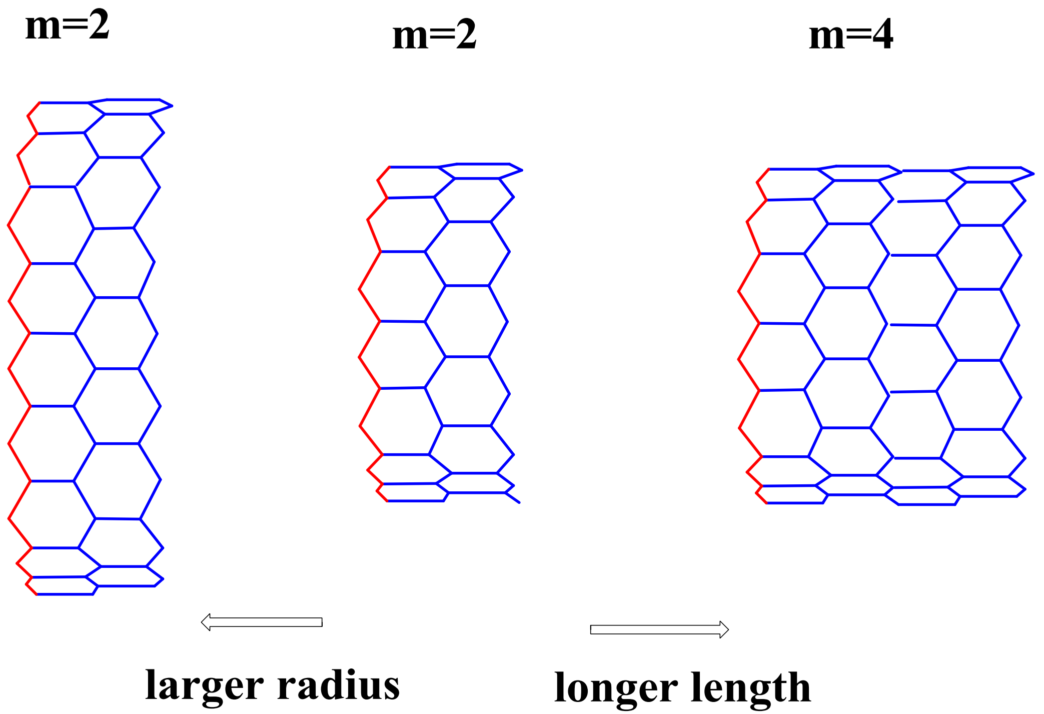
n=14



HOMO-LUMO gaps

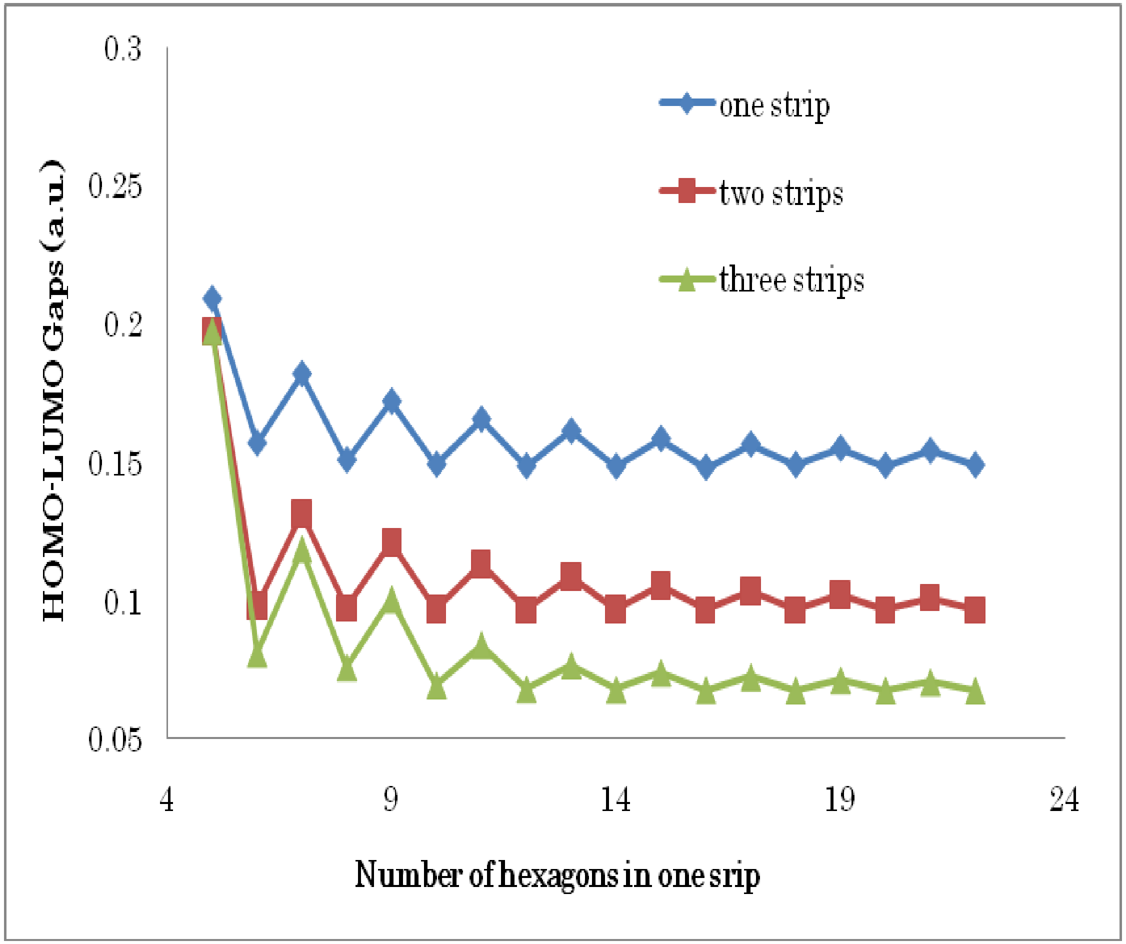
The HOMO-LUMO gaps of this series of molecules decease monotonically with the increase of the number of hexagons in the systems.

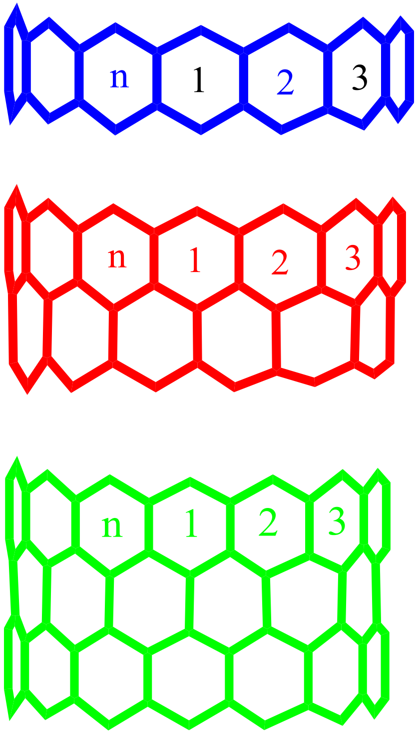
The electronic properties of $(n,0)_m$ may change drastically with increase of the size of tubes, larger radius or longer length. Here $(n,0)_m$ denotes finite-length zigzag carbon nanotubes with m layers



Zigzag nanotubes with different radius or different length

If we make zigzag carbon nanotubes longer, then HOMO-LUMO gaps decease monotonically .
However it was shown that the HOMO-LUMO gaps of zigzag CNTs oscillate with an odd or even number of hexagons in the circular plane of the nanotube.

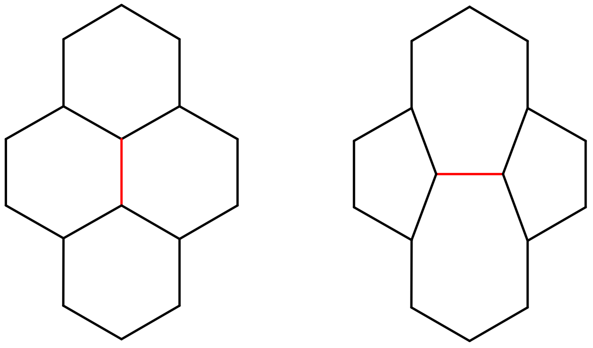




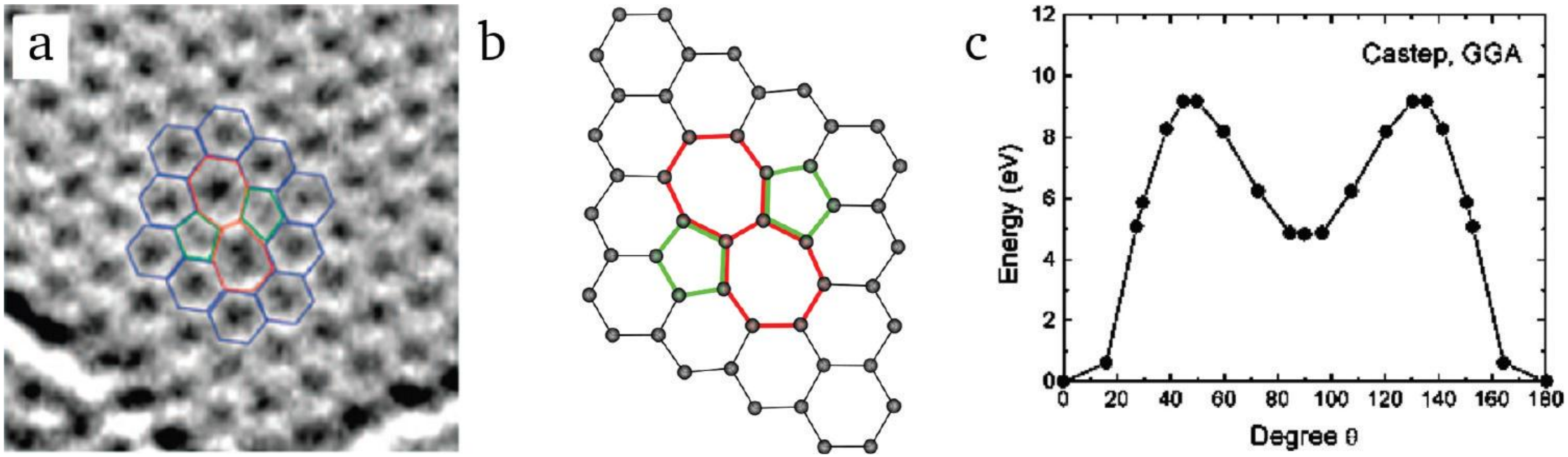
Stone-Wales Defect

Various kinds of defects are known to be present in carbon nanotubes, which have significant influence on electronic, mechanical, and transport properties of the tubes.
The Stone-Wales defect plays a key role, enabling large-scale structural rearrangements in graphitic networks.

A 90 degrees bond rotation in a hexagon network leads to the formation of two pentagons and two heptagons.



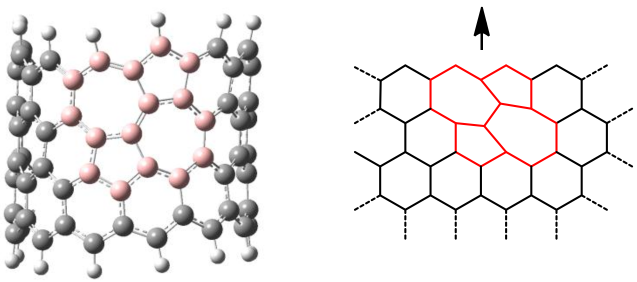
Stone-Wales Defect



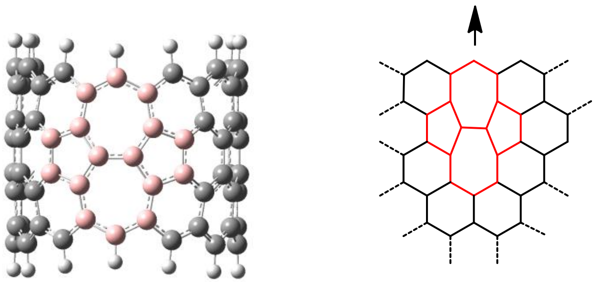
a) Experimental TEM image of the defect,
b) its atomic structure as obtained from our DFT calculations

J. Meyer, 2008

There are two types of configurations of Stone-Wales defects in zigzag carbon nanotubes, H-type and V-type as shown below



H-type

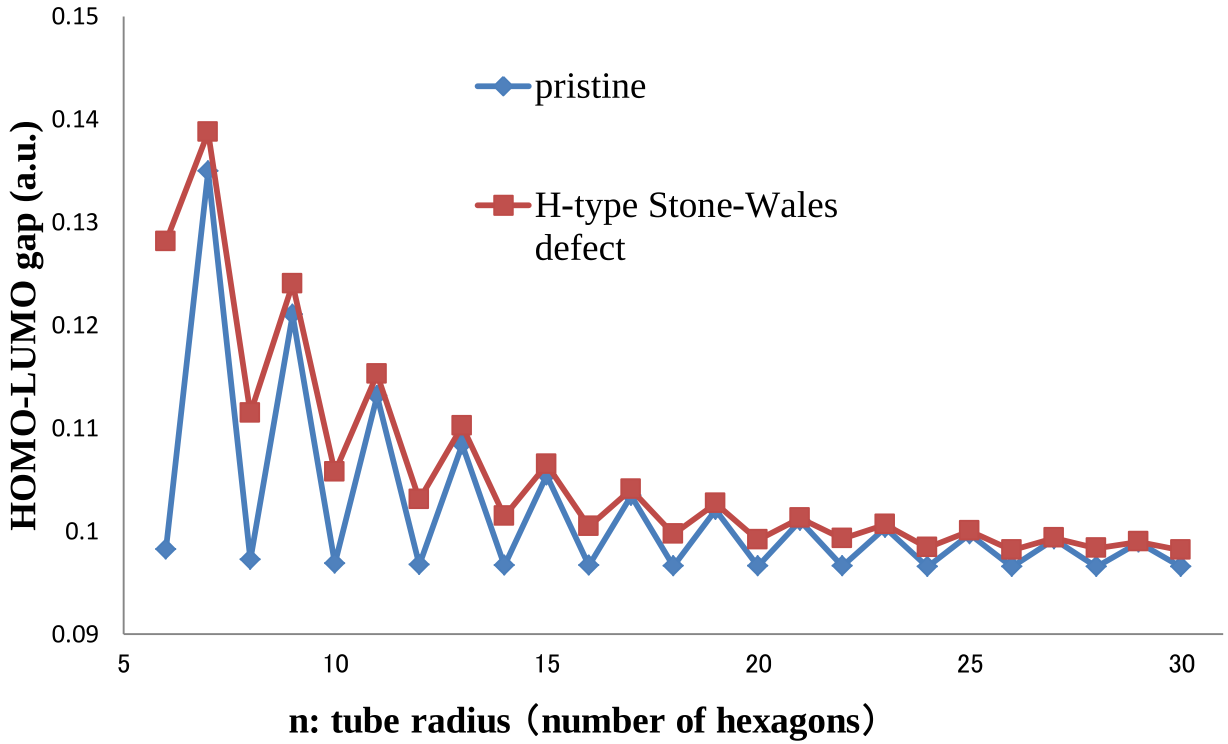


V-type

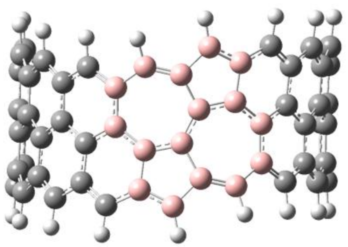
The purpose of this paper is to study the effects of Stone-Wales defect on the HOMO-LUMO gap oscillation in $(n,0)_m$ zigzag carbon nanotube. We used PM3 method.

2. Effect of SW defect on HOMO-LUMO gaps

HOMO-LUMO gaps in Zigzag CNTs with SW defect



two layers

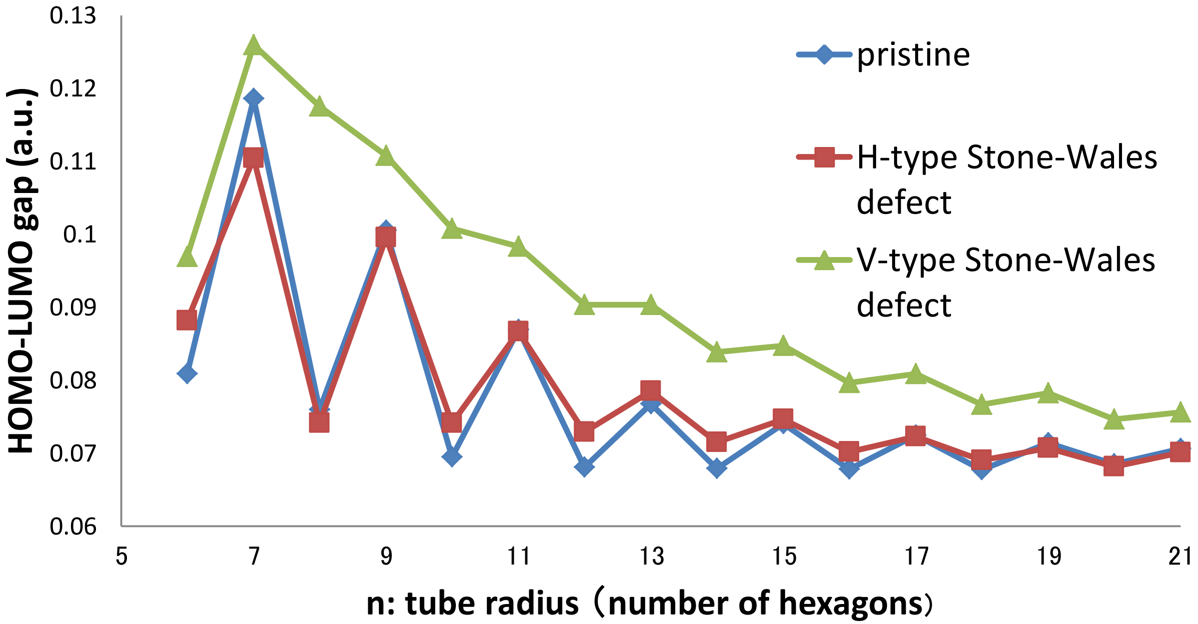


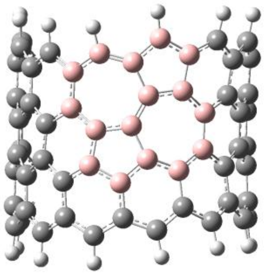
H-type

The HOMO-LUMO gaps in zigzag CNTs with SW defect show the oscillation depending on the number of hexagons around the peripheral circuits.

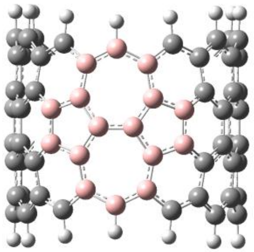
HOMO-LUMO gaps in Zigzag CNTs with SW defect

three layers





H-type



V-type

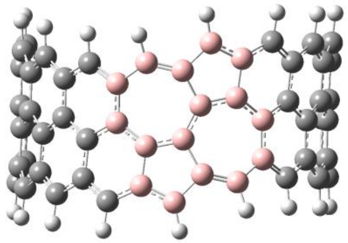
Regardless of the types of the configurations of Stone-Wales defect , the HOMO-LUMO gaps in zigzag CNTs with SW defect oscillate with period 2.

The HOMO-LUMO gaps in zigzag CNTs with V-type SW defect are larger than those in pristine CNTS.

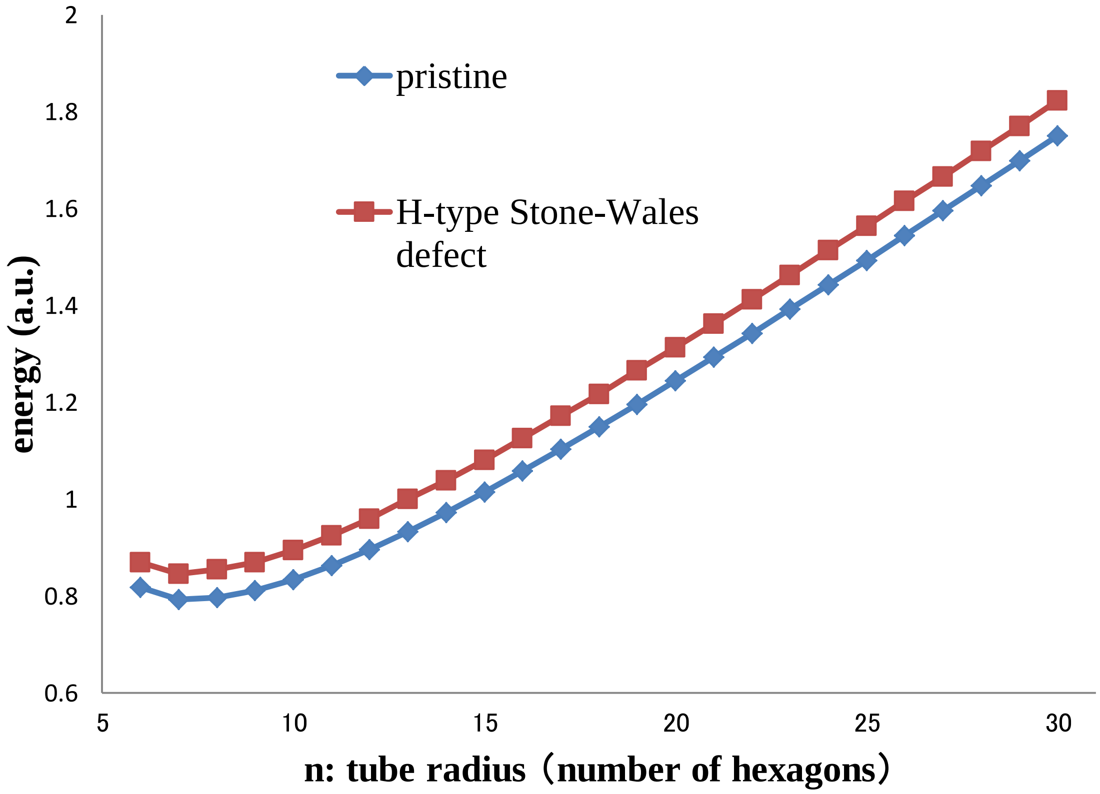
The HOMO-LUMO gaps in zigzag CNTs with H-type SW defect are almost the same as those in pristine CNTS.

Energies of Zigzag CNTs with SW defect

This figure shows the dependence of the total energies of zigzag CNTs on the radius of tubes.



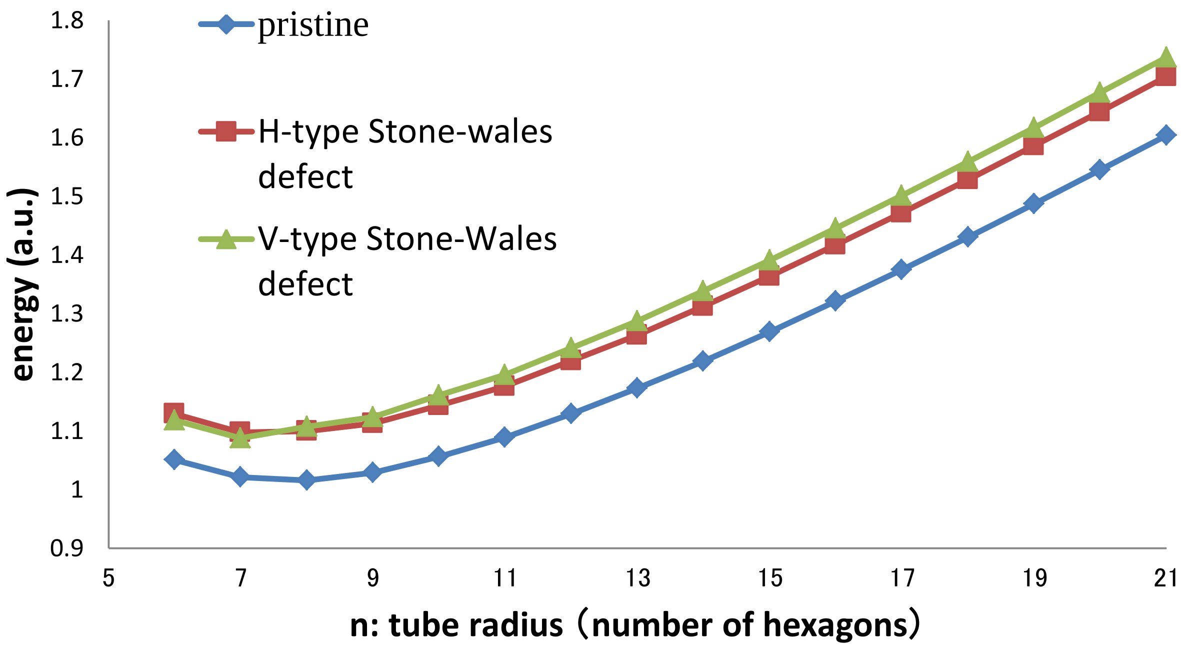
H-type
two layers

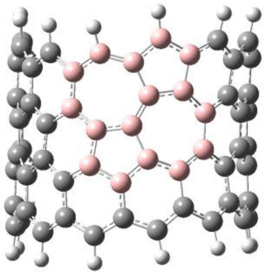


Zigzag CNTs with SW defect are more unstable than pristine zigzag CNTs.

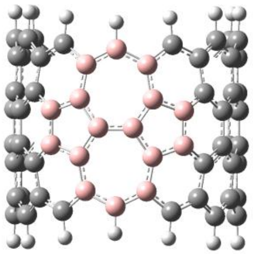
Energies of Zigzag CNTs with SW defect

three layers





H-type



V-type

Regardless of the types of the configurations of SW defect , zigzag CNTs with SW defect are higher in energy than pristine zigzag CNTs.
Zigzag CNTs with SW defect of H-type are slightly lower in energy than zigzag CNTs with SW defect of V-type .

3 Conclusions

By using PM3 method we found that

1) the HOMO-LUMO gaps in zigzag CNTs with SW defect oscillate with an odd or even number of hexagons in the circular plane of the nanotube.

2) the HOMO-LUMO gaps in zigzag CNTs with SW defect are larger than those in pristine CNTS.

3) zigzag CNTs with SW defect are higher in energy than pristine zigzag CNTs.

The HOMO−LUMO gap is an indicator of kinetic stability.
The total energy is an indicator of the thermodynamic stability.

From 2 and 3 we can say that

zigzag CNTs with SW defect are chemically more stable but thermodynamically more unstable than pristine zigzag CNTs.

Thank you for your attention.