Electronic structure of polyicosahedral silicon nanostructures.

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In a previous molecular dynamics study[1,2], we predicted a polyicosahedral Si nanostructure which composed of linked icosahedral Si nanodots. In this presentation[3], we report on a first-principles study of the electronic structure of hydrogenated polyicosahedral Si nanostructures; icosahedral $Si_{100}H_{60}$ nanodot, polyicosahedral $Si_{175}H_{90}$ nanodot, and polyicosahedral $Si_{150}H_{60}$ nanowire. All the calculations are carried out by the density functional theory within the local density approximation using the OpenMX code[4].

Our results show that the band gap energy increases from 1.20, 1.60 to 2.09 eV, as the number of linked icosahedra decreases from ∞ ($Si_{150}H_{60}$ nanowire), 2 ($Si_{175}H_{90}$ nanodot) to 1 ($Si_{100}H_{60}$ nanodot) due to the quantum confinement effect. The analyses of electronic wave functions reveal that the wave functions of the polyicosahedral nanodot and polyicosahedral nanowire can be expressed as linear combination of wave functions of the icosahedral nanodot. In Fig. 1, we compare the electronic band structure of the polyicosahedral nanowire with that of similar-size pentagonal $Si_{30}H_{10}$ nanowire and crystalline diamond $Si_{45}H_{20}$ nanowire. We find that the band gap energy and the effective masses of Si nanowires strongly depend on the arrangement of Si atoms. On the basis of these results, we suggest that the size and the atomic arrangement play an important role in determining the electronic properties of Si nanostructures.

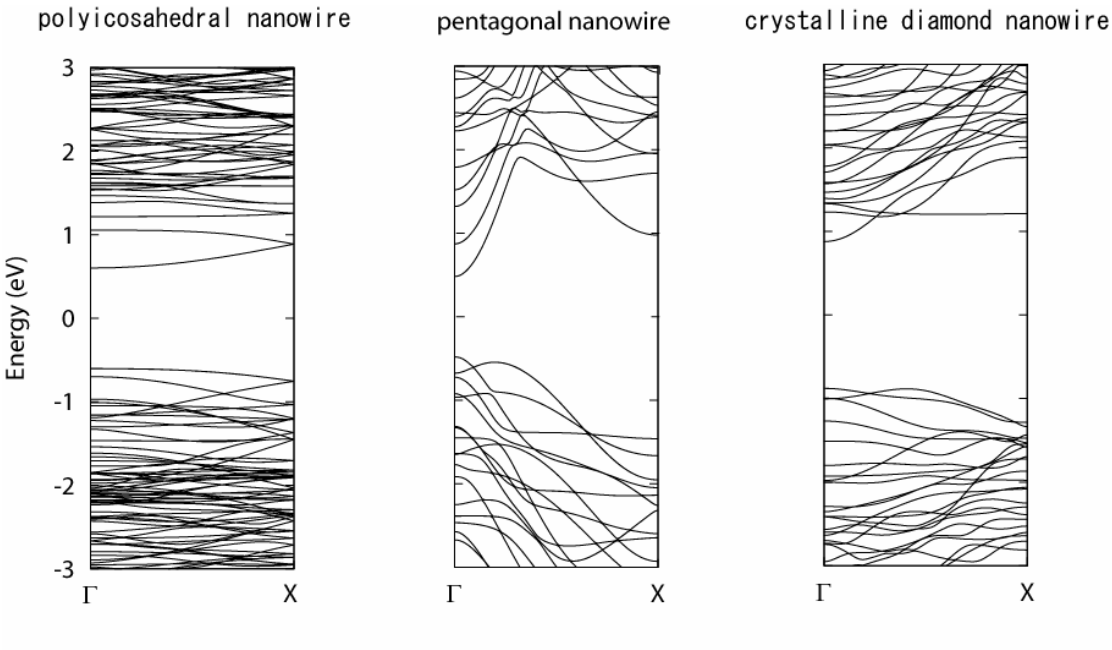

Figure 1: Electronic band structures of similar-size Si nanowires.

[1] K. Nishio et. al., J. Chem. Phys.**125**, 074712 (2006).
[2] K. Nishio et. al., Phys. Rev. B **72**, 245321 (2005).
[3] K. Nishio et. al., submitted to Phys. Rev. B
[4] http://www.openmx-square.org/