First-Principles Calculations of Electronic and Transport Properties of Nanowires

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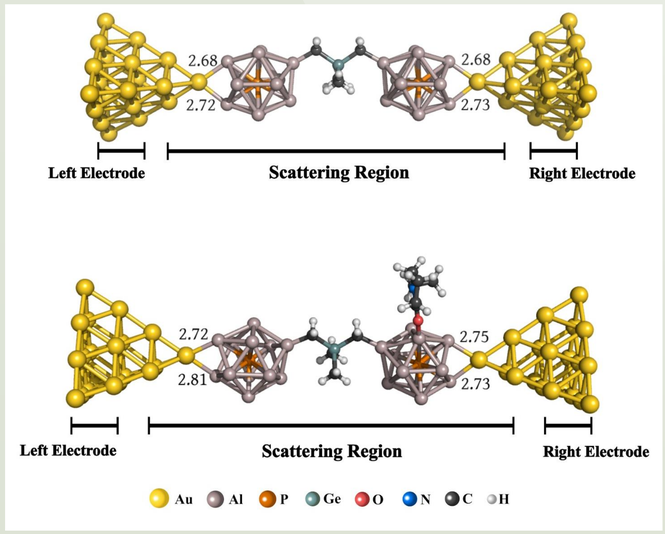
Abstract

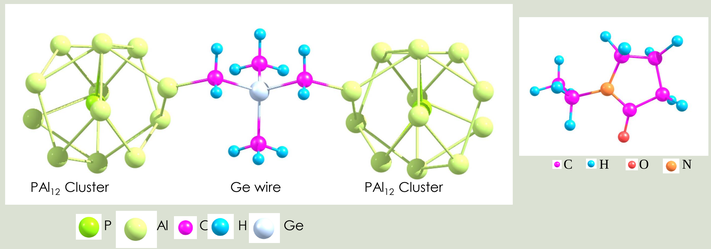
The goal of this research is to find out the electronic structure and transport property of nanowires (NWs) that we are interested in. As Moore's law is faltering, scientists are trying to use different methods to continue to increase computer's computing power like using carbon nanotubes or quantum transistors. In the spirit of this, semiconducting nanowires constituted of atomic units and choices of ligands are proposed to mimic the functions of transistors to achieve the goal of increasing computing power. Electronic structure and electron transport calculations have been conducted based on the density function theory and the non-equilibrium Green's function (NEGF) method to show the effect of ligands on the nanowire.



Schematic illustration of transport setup: nanowire structure with and without a ligand

Objectives

The nanowire that will be studied is composed of two PAl_{12} Clusters linked by a Ge wire (GeC_4H_{10}):



- Calculate the electronic structure of the nanowire
- Analyze the transport property of the nanowire
- Study the effect of ligands on these properties of nanowires

Computational Methods

For the electronic structure calculation:

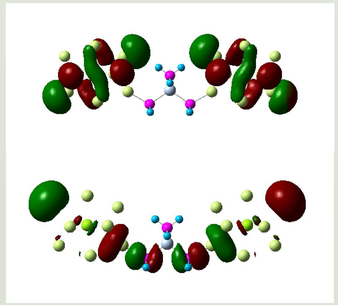
- Density Functional Theory
  - Gaussian 09
  - Exchange correlation functional: PBE
  - Basis sets: 6-31G(d.p)
  - Molecular orbital (MO)

For the electron transport calculation:

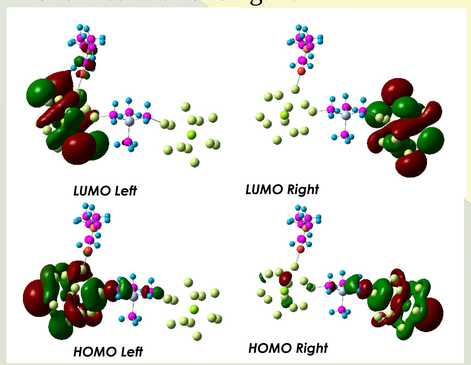
- Non-Equilibrium Green's Function (NEGF) method
  - Siesta / TranSiesta
  - Exchange correlation functional: PBE
  - Basis sets: DZP with pseudopotential
  - Transmission function
  - Projected density of state (PDOS)
  - Local density of state (LDOS)

Results

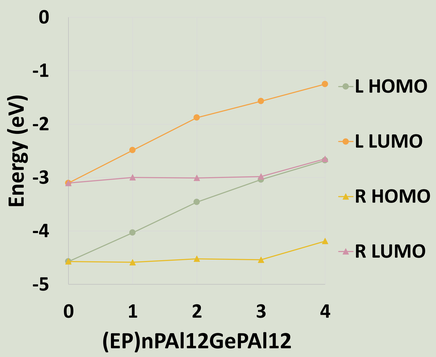
HOMO and LUMO of a NW with no ligand



Projected HOMO and LUMO of a NW with one ligand

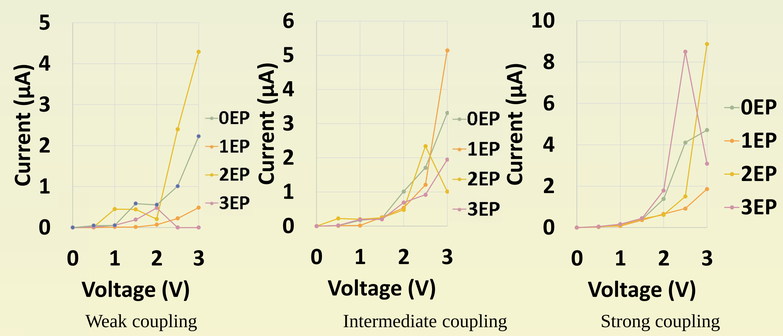


Effect of Ligand: HOMO-LUMO gap chart as the number of ligands increases

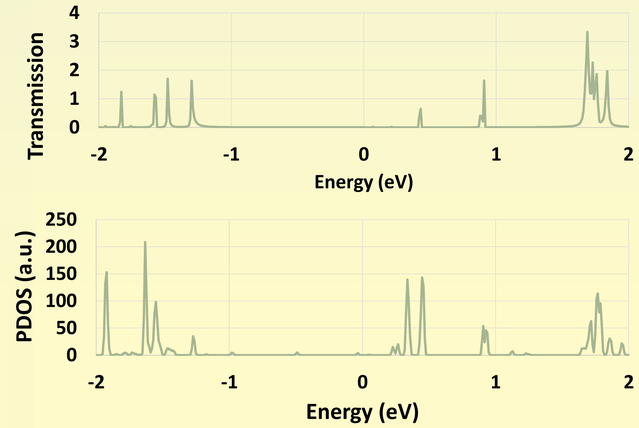


	Left		Right	
	HOMO	LUMO	HOMO	LUMO
EP0	-4.57	-3.10	-4.57	-3.10
EP1	-4.03	-2.49	-4.59	-3.00
EP2	-3.46	-1.88	-4.52	-3.01
EP3	-3.04	-1.57	-4.43	-2.98
EP4	-2.68	-1.25	-4.19	-2.65

Current vs. Voltage of Strong/ Intermediate/ Weak coupling



Transmission vs. energy and PDOS vs. energy



Conclusions

Based on electronic structure calculations, there are three properties of the nanowire is found:

- First, the nanowire structures are stable;
- Second, adding ligands makes the MOs localized;
- Third. increasing the number of ligands decrease the HOMO-LUMO gap.

Based on electron transport calculations,

- For the one-ligand case, its current over 0 - 3 V is smaller than that of the no-ligand case, even though the HOMO-LUMO gap becomes smaller.
- For the two- or three-ligand case, the current becomes higher over certain voltages, which means the smaller HOMO-LUMO gap overcomes the drawback of localized molecular orbitals.