Abstract of Presentation

Presentation Title:

Computational nano-materials design and its application to spintronics

Abstract :

The development of the basic technology strongly relies on the physical science as well as materials science. In order to respond the ever-increasing demand for materials with required properties and functionalities, methods free from energy consumption and environmental problems are necessary. One of the most powerful methods that meet this requirement is *computational nano-materials design* (CMD). CMD is the method that synthesizes new materials at a virtual laboratory in a computer. The key machinery of this process is called *computational materials design engine*. The computational materials design engine composed of a three-step iteration cycle. The first step is a quantum simulation, the second one is the step finding a mechanism behind, and the last one is a guess of new systems. These steps are iterated until finally we find a new material that possesses the required properties. In such a way we can solve the inverse problem of quantum simulations: Namely, given properties, we predict a material that exhibits the desired properties. Note that, the quantum simulation merely predicts properties of given material. In this talk, we give an example of CMD to illustrate the way it works.

The first topic is the spin injection and accumulation associated with a DC current in a GMR geometry. We considered a ferromagnetic/nonmagnetic interface, for example, a Co/Cu interface, and calculated the DC conductivity using the Korringa–Kohn–Rostoker (KKR) Green's function method combined with the Kubo–Greenwood formula. The full spin-orbit coupling is taken into account in order to take account of the spin relaxation. The obtained conductivities are discussed in connection with the electronic structure at the Fermi level. From the calculated conductivities, we estimated the spin injection and accumulation by use of a Boltzmann-type phenomenological discussion. We also drew a picture of the electrochemical potential of the ferromagnetic/ nonmagnetic interface. From these results, we found that rather big spin injection and accumulation could occur in the case of the Co/Cu interface.

The second topic is the design of half-metallic antiferromagnets (HM-AF). HM-AF could be more useful than half-metallic ferromagnets in spintroics devices since they are insensitive to external fields and also injection of spins is rather easy owing to their small shape magnetic anisotropy. Such a type of half-metal is possible when the system is composed of two types of different magnetic ions whose total d-electron number is ten. We have designed several types of HM-AF's. The examples are (ZnVCo)S and $CrFeS_2$. The former is a diluted magnetic semiconductor and the latter is an intermetallic compound. The calculation showed that both of them exhibit clear AF-HM features.