Electronic properties of molecular solids and Beyond - Toward to Bio-Materials Science

Hidetoshi Fukuyama
Tokyo University of Science, Kagurazaka, Shinjuku-ku 162-8601, Tokyo
E-mail; fukuyama@rs.kagu.tus.ac.jp

The electronic properties of molecualr solids are truly diverse reflecting variety of molecules involved and possible spatial arrangement of molecules in unit cell of crystals. One of the main interests in molecular solids is the realization of conductors, especially superconductors, which have been achieved through synthesis of charge transfer solids, where two different kinds of molecular are arranged in crystal.[1] A recent highlight in studies on molecular conductors is the realization of single component molecular metals where metallic states are realized by just one kind of molecule.[2]

Theoretically it appeared at first stage impossible even to try to understand the origin of electronic properties of each molecular conductor on a microscopic basis because of the complex atomic arrangements and expected complicated electronic states. It turned out, however, that the straightward and systematic understanding of electronic properties of molecular solids are now possible. This is due to the fact that the tight-binding approximation based on molecular orbilal is basically valid.[3] At the same time the effects of Coulomb interaction among electrons and those with phonons, which are driving forces of various ground states and associated phase transitions, can be microscopically addressed based on the theoretical model (extended Hubbard model), which is familiar in conventional theories of solids.[4]

It is interesting to observe that there are a few molecular conductors, where the metallic ions are imbedded in π electrons of molecules, which are termed "π-d systems". Actually the above-mentioned single component molecular metals belong to this category and have transition metal ions at the center strongly mixing with the π - states of side units of the molecule. The local atomic arrangement in such π-d systems shares the same feature with that of active centers of typical proteins, e.g. myoglobin, where various electronic processes take place at Fe ions (Fe^{+2} and Fe^{+3}, together with high and low spin states). In this case detailed understanding of the relationship between local structure (distortion) around active centers and associated electronic states (especially energy levels) will naturally lead to the understanding of functionalities of proteins on very firm basis not immediately but eventually. Likewise there are cases in bio-related materials where electronic processes may be studied in ways similar to those in condensed matter science, which may be classified as [5] [1] Active centers in proteins such as (a) metal ions, e.g. both heme and non-heme, (b) clusters, e.g. Fe_4S_4, (c)functional molecules, e.g. retinal in rhodopsin, and [2] DNA.

To address these challenges is not easy because there are many different and important aspects in each problem and then collaborations among experts in different disciplines are crucially important. This meeting is organized just for this ; i.e. to exchange of modern knowledge among different disciplines leading to the basis of *Bio-Materials Science.*

[1] Various papers in *Chemical Reviews,* **104** (2004) #11.
[2] H. Tanaka et al., *Science* **291** (2001) 285; A. Kobayashi, E. Fujiwara and H. Kobayashi, *Chemical Reviews*, **104** (2004) 5243.
[3] T. Mori et al., *Bull Chem. Soc. Jpn.*, 57 (1984) 627, and references cited therein.
[4] H. Seo, C. Hotta and H. Fukuyama, *Chemical Reviews* 104 (2004) 5005.
[5] H. Fukuyama, J. Phys. Soc. Jpn., 75 (2006) 051001.