



SPEAKER

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First-principles investigation on the electronic states of the organic single-crystals and the organic-metal interfaces: importance of accurate prediction of the crystal and the interface structures

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@ Meeting Room C015, Lab 1

Abstract: These years, there has been enormous attention paid to development of organic semiconductor materials for next-generation flexible electronics. To enhance the performances and the functions of the materials, more understanding on the materials properties at the nano-scale size is required. There have been more and more efforts made to understand the electronic properties of the organic materials both experimentally and theoretically.

In this talk, I will present my recent theoretical works on the electronic properties of the organic solids. I focus on the two topics:

- i) Interface dipole dominating the energy level alignment at the organic-metal interface: pentacene-metal and Alq₃-metal interfaces as examples
- ii) Band structure and its dispersion of organic single crystals and its origin: cases of rubrene and metal-phthalocyanine

The former topic is related to the formation of the charge injection barrier right at the organic-electrode interface, and the latter one is to the recently proposed band-like carrier transport in organic semiconductor single crystals.

For theoretical calculations, I employ the density functional theory (DFT) to predict the structural and electronic properties of the materials. I also use recently proposed variants of DFT to take into account the van der Waals (vdW) interaction dominating the intermolecular and the molecule-substrate interactions.

The importance of the accurately predicted crystal and interface structures will be highlighted, and I will discuss the effects of the structures on the electronic properties.



References

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[3] S. Yanagisawa, Y. Morikawa, and A. Schindlmayr, Phys. Rev. B 88, 115438 (2013).

[4] S. Yanagisawa, K. Yamauchi, T. Inaoka, T. Oguchi, and I. Hamada, Phys. Rev. B 90, 245141 (2014).

Biography:

Education record

PhD, Department of Applied Chemistry, School of Engineering, University of Tokyo, Japan, 2004; Supervisor: Professor Dr. Kimihiko Hirao

Work Experience

October 2003-March 2004

Postdoctoral fellow, Intelligent Modeling Laboratory, University of Tokyo

April 2004-September 2009

Postdoctoral fellow, Institute of Scientific and Industrial Research, Osaka University

October 2009-March 2011

Postdoctoral fellow, Department of Precision Science and Technology, Osaka University

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Assistant Professor, Department of Physics and Earth Sciences, Faculty of Science University of the Ryukyus

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