

Organic molecules on surfaces: from static towards dynamic pictures

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The interaction between organic molecules and solid surfaces play a pivotal role in not only surface chemistry [1, 2] but also surface physics and nano-science [3]. In the former case, surface scientists have microscopically elucidated how chemistry works at surfaces including catalysis using various spectroscopic and microscopic methods. In the latter case, the recent developments of organic electronic devices such as organic light emitting diodes, organic field-effect transistors and photovoltaic cells are spectacular. The further improvement and innovations require an in-depth understanding of both electronic states and structures at organic-metal or organic-organic interfaces [4].

In this talk, I will present two topics in our recent studies. One is the interaction between cyclohexane and Rh(111) [5]. The hydrogenation/dehydrogenation of hydrocarbon molecules on a transition metal surface is typical catalytic reactions. Vibrational spectra of alkanes adsorbed on metal surfaces often show the presence of significantly red-shifted and broadened C-H stretching bands, called as the “soft mode.” The soft mode has been attributed to the C-H bonds directly interacting with metal surfaces. Hence, elucidation of the softening mechanism is essential to understand the interaction between alkanes and metal surfaces, and the reaction processes of heterogeneous catalysis. Secondly, the adsorption and electronic states of tetrafluoro-tetracyanoquinodimethane (F4-TCNQ) on Cu(100) is discussed [6]. F4-TCNQ showing a high electron affinity ($E_A = 5.24$ eV) has been studied on various substrates from the perspective of the p-type doping of organic films, the energy level alignment on metal surfaces [7], and the surface transfer doping of semiconductor surfaces [8]. In the case of F4-TCNQ on Cu(100), the local interaction between cyano groups and surface Cu atoms plays a more important role than just a simple charge transfer from the Cu substrate to F4-TCNQ; not only the rearrangements of surface Cu atoms occur, but also F4-TCNQ is highly perturbed from a planar structure.

References

- [1] G. Ertl, “Reactions at Solid Surfaces” (Wiley, 2009).
- [2] G. A. Somorjai and Y. Li, “Surface Chemistry and Catalysis, 2nd ed.” (Wiley, 2010).
- [3] R. Waser (ed.), “Nanoelectronics and Information Technology” (Wiley-VCH, 2005).
- [4] J. Fraxedas, “Molecular Organic Materials” (Cambridge, 2006).
- [5] T. Koitaya, A. Beniya, K. Mukai, S. Yoshimoto and J. Yoshinobu, Phys. Rev. B 80 (2009) 193409.
- [6] T. Katayama, K. Mukai, S. Yoshimoto and J. Yoshinobu, J. Phys. Chem. Lett. 1(2010) 2917.
- [7] S. Braun and W. R. Salaneck, Adv. Mater. **21**, 1450 (2009).
- [8] W. Chen, D. Qi, X. Gao, and A. T. S. Wee, Prog. Surf. Sci. **84**, 279 (2009).