

平成 24 年 5 月 14 日

応用物理学会北海道支部
会員各位

応用物理学会北海道支部講演会のお知らせ

下記講演会を開催いたしますので、多数ご参加下さいますようご案内申し上げます。

演題： Dynamic structure of supported Pt and Pt-Sn nanoclusters

講師： John J. Rehr 氏

(Department of Physics, Washington University, Professor)

日時： 平成 24 年 7 月 9 日 (月) 16:00~17:30

場所： 北海道大学 創成科学研究棟 4 階 セミナー室 B, C

共催： 応用物理学会北海道支部, 触媒化学研究センター (申請中), 日本化学会北海道支部 (申請中), 触媒学会北海道支部 (申請中)

講演の要旨

The nature of local atomic and electronic structure at the nanoscale is of both fundamental and technological importance. These local and generally dynamical properties are especially important for understanding the role of supported metal clusters, which are key ingredients in many catalytic processes. Understanding these properties thus requires real-time approaches, which are becoming increasingly important in studies based on x-ray absorption spectra (XAS). In this talk I will discuss a real-time approach for calculating dynamic structure based on *ab initio*, finite-temperature density functional theory/molecular dynamics and the real-space Green's function approach for XAS calculations based on the FEFF9 code [1]. This approach exploits recent theoretical advances that permit parameter-free calculations of the key many-body effects in the theory. This method is illustrated for nano-clusters of Pt [2] and Pt-Sn [3] supported on gamma-alumina. The simulations reveal a complex, non-equilibrium structure on multiple-time scales, including a hindered Brownian motion of the center of mass and fluctuating bonding. In particular their internal structure varies dynamically on a time scale of a few ps. Charge transfer between atoms in the cluster and between the cluster and the surface are particularly important. These results explain many unusual properties observed for supported Pt nanoclusters including large temperature dependence, anomalous disorder, and negative thermal expansion. For Pt-Sn, the simulations show that the Sn atoms are especially mobile, but the clusters still have well defined Pt-Pt and Pt-Sn coordination shells, and between 2 – 5 bonds between Pt or Sn atoms in the cluster and the O atoms at the surface. Simulations of the XANES are observed to be in reasonable agreement with experiment demonstrating the importance of taking into account the large, internal fluctuations in these structures. Implications for bonding and catalytic properties are also briefly discussed.

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[1] J. J. Rehr, J. J. Kas, M. P. Prange, A. P. Sorini, Y. Takimoto, and F. Vila, *Comptes Rendus Physique*, 10, 548 (2009).

[2] F. Vila, J. J. Rehr, J. Kas, R. G. Nuzzo, and A. I. Frenkel, *Phys. Rev. B* 78, 121404(R), (2008).

[3] F. Vila, J. J. Rehr, S. D. Kelly, and S. R. Bare, *Bull. Am. Phys. Soc.* (2011).

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J. J. Rehr 先生は、XAFS 理論を長年研究され、XAFS 解析手法として広く使われる FEFF の開発者であります。この 10 年、触媒やナノ粒子の XAFS の理論解析に興味を持たれています。せっかくの機会ですので、多くの方の参加を期待しております。