Metal-insulator transitions: a real space picture

Alexey I. Baranov, Miroslav Kohout, Max-Planck Institute for Chemical Physics of Solids, Dresden (Germany). E-mail: baranov@cpfs.mpg.de

Traditionally the metals and insulators are distinguished by different filling of their electronic bands implying thus an analysis in k-space. Electron localization indices (LI) showing the degree of electron pair exchange inside/between various regions of space represents an attractive alternative to analyze the electronic motion in real space [1]. Recently these indices have been made available also for solids which open new opportunities for the analysis of their electronic structure [2]. We have applied the LI to two different metal-to-insulator transitions in the current study.

First one is the observed experimentally pressure-induced transition of sodium metal having the double-hcp structure (Pearson symbol hP4) into transparent insulating solid [3]. It is found that the LI for QTAIM [4] and ELI-D [5] basins show different picture of electronic motion than for the metallic phase.

Another transition is a representative of large and very important class of Mott transitions which are driven by strong electronic correlation effects. A model system of 1D hydrogen chain calculated with spin-polarized DFT was selected for the study which provided correlation effects. A model system of 1D hydrogen chain calculated class of Mott transitions which are driven by strong electronic

where \( P_x \) is the degree of circular polarization of incident x-rays, \( S \) the spin direction, \( \mathbf{k} (\mathbf{k}') \) the wavevector of incident (scattered) x-rays, \( \theta \) the scattering angle. \( C \) and \( C_{\text{mag}} \) are constants. The first term contains the charge Compton profile \( J(p_z) \) and the second term the magnetic Compton profile \( J_{\text{mag}}(p_z) \). They are given by,

\[
J(p_z) = \int [n_{\uparrow}(p_z) + n_{\downarrow}(p_z)] \, dp_y \, dp_z - J_{\uparrow}(p_z) + J_{\downarrow}(p_z) \tag{2}
\]

\[
J_{\text{mag}}(p_z) = \int [n_{\uparrow}(p_z) - n_{\downarrow}(p_z)] \, dp_y \, dp_z - J_{\uparrow}(p_z) - J_{\downarrow}(p_z) \tag{3}
\]

where \( n_{\uparrow}(p_z) \) and \( n_{\downarrow}(p_z) \) are the electron momentum densities, and \( J_{\uparrow}(p_z) \) and \( J_{\downarrow}(p_z) \) are the Compton profiles for up- and down-spin states. \( p=(p_x, p_y, p_z) \) is the electron momentum. Both \( J(p_z) \) and \( J_{\text{mag}}(p_z) \) are accessible to Compton scattering techniques, and once the both profiles are normalized the spin-wise decomposed Compton profiles, \( J_{\uparrow}(p_z) \) and \( J_{\downarrow}(p_z) \), are obtained through eqs. (2) and (3) [1].

In this presentation we demonstrate the feasibility of this method by showing its application to ferromagnetic manganites \( \text{La}_{1-x}\text{Sr}_{x}\text{MnO}_3 \) [2].

Keywords: metal_insulator_transition, density_functional_theory, electronic_localization_indices

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**Microsymposia**

**MS.48.4**


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**MS.49.1**


**Molecular-scale 3D visualization of solid-liquid interfaces by FM-AFM**

Hirofumi Yamada,* Kazuhiro Suzuki,† Noriaki Oyabu,* Kei Kobayashi,* Department of Electronic Science and Engineering, Kyoto University, *Office of Society-Academia Collaboration for Innovation, Kyoto University, Kyoto (Japan). E-mail: h-yamada@kuee.kyoto-u.ac.jp

Solid-liquid interfaces play essential roles in a wide variety of physical and chemical processes, such as crystal growth, electrochemical reactions and various biological functions. Investigations of atomic-scale structures and interactions at solid-liquid interfaces are, therefore, essentially important for understanding theses microscopic processes. Force mapping method based on frequency modulation atomic force microscopy (FM-AFM) is a remarkable technique for atomic-scale investigations of interaction forces on a specific site of crystal surfaces. The technique has been used mainly in vacuum environments, where highly sensitive force detection can be performed due to the high Q-factor in the cantilever oscillation. However, since significant progress has been made in FM-AFM in liquids over the past few years [1, 2], the force mapping method can be used for atomic or molecular scale investigations of interaction forces at solid-liquid interfaces, such as solvation forces.

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