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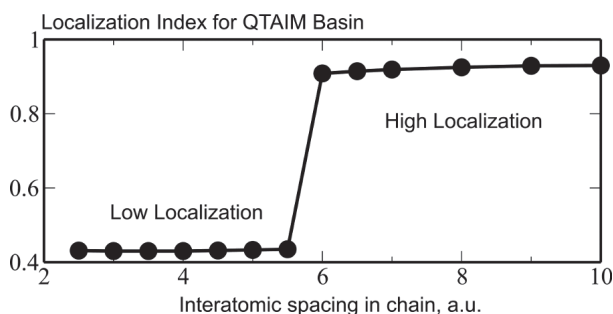
Metal-insulator transitions: a real space picture

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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 qualitatively acceptable description of Mott transition for this case. A metal to insulator transition is reproduced as an abrupt increase of LI value for the QTAIM basin of hydrogen atom (see Fig.)



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Spin-wise decomposed compton profiles

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$$\frac{d^2\sigma}{d\Omega d\omega} = C \cdot J(p_z) + C_{mag} \cdot P_C \cdot \mathbf{S} \cdot (\mathbf{k} \cos\theta + \mathbf{k}') J_{mag}(p_z), \quad (1)$$

A spin-polarized electronic state dominates the magnetic properties

of materials and is decomposed into the up- and down-spin electronic states in a non-relativistic treatment. The spin-polarized state such as magnetization density is a central subject of magnetism and has been studied on various magnetic materials by neutron and X-ray scattering techniques. In this study we propose a method to decompose the spin-polarized state into the corresponding up- and down-spin states by a Compton scattering technique. This method provides unique information on the transport and magnetic properties of half-metallic materials.

When the incident x-rays are circularly polarized, the cross section for Compton scattering is given by,

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

$$J(p_z) = \iint [n_{up}(\mathbf{p}) + n_{down}(\mathbf{p})] dp_x dp_y = J_{up}(p_z) + J_{down}(p_z), \quad (2)$$

$$J_{mag}(p_z) = \iint [n_{up}(\mathbf{p}) - n_{down}(\mathbf{p})] dp_x dp_y = J_{up}(p_z) - J_{down}(p_z), \quad (3)$$

where $n_{up}(\mathbf{p})$ and $n_{down}(\mathbf{p})$ are the electron momentum densities, and $J_{up}(p_z)$ and $J_{down}(p_z)$ are the Compton profiles for up- and down-spin states. $\mathbf{p}=(p_x, p_y, p_z)$ is the electron momentum. Both $J(p_z)$ and $J_{mag}(p_z)$ are accessible to Compton scattering techniques, and once the both profiles are normalized the spin-wise decomposed Compton profiles, $J_{up}(p_z)$ and $J_{down}(p_z)$, 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].

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

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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 these 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.