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Electron Momentum Density: Recent Progress and Perspective for Combined Studies

Y. Sakurai¹

¹Japan Synchrotron Radiation Research Institute, Sayo Hyogo, Japan

Quantum mechanical descriptions are becoming a focus of attention in understanding the behavior of wide classes of materials. This paper discusses some of our recent works related to charge or magnetic Compton scattering studies. Selected topics include: (1) Quantum modelling of doped holes in high-Tc cuprates [1], which provides insight into the dome-shaped doping dependence of the superconducting transition temperature. (2) Analyses of Compton scattering X-ray spectra in spin-crossover cobaltates, which allows us to delineate the t2g-eg physics and quantum chemistry from the temperature evolution of electron momentum density. As a conclusion remark, we show an example of combined studies [2] and present its perspective, emphasizing that X-ray Compton scattering is highly sensitive to delocalized or itinerant electrons.

[1] Y. Sakurai et al., Science, 2011, 332, 698-702., [2] N. Qureshi et al., Phys. Rev. B, 2009, 79, 094417.

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