Contribution ID: **248** Type: **Poster presentation**

The Role of Core Hole Effects on Calculated Resonant Inelastic X-Ray Scattering Spectra of Graphene

Thursday, 21 May 2015 08:00 (3 hours)

The electronic band structure of graphene was calculated using the full-potential linearized muffin-tin orbital (FP-LMTO) method. Its resonant inelastic x-ray scattering (RIXS) spectra at various x-ray excitation energies were calculated based on Kramers-Heisenberg equation. It is found that the RIXS spectra show distinct dispersive features and are interpreted as being due to the conservation
of crystal momentum during the RIXS process. However, the shift between XAS and XES energy scales due to the presence or absence of the core hole in the final state of these two processes, respectively, has to be taken into account, in order to obtain an optimal agreement between the simulated and experimental RIXS spectral. This shift is consistent with the observed changes in
calculated PDOS induced by the presence of the core hole.

Summary

Primary author: SCHWERTFAGER, Nuchalee (School of Physics and NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand; Thailand Center of Excellence in Physics (ThEP Center), Commission on Higher Education, Bangkok 10400, Thailand)

Co-authors: Prof. ZHANG, Liang (National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei 230029, China; Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA); Prof. LIMPIJUMNONG, Sukit (School of Physics and NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand; Thailand Center of Excellence in Physics (ThEP Center), Commission on Higher Education, Bangkok 10400, Thailand); Prof. LAMBRECHT, Walter (Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106-7079, USA)

Presenter: SCHWERTFAGER, Nuchalee (School of Physics and NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand; Thailand Center of Excellence in Physics (ThEP Center), Commission on Higher Education, Bangkok 10400, Thailand)

Session Classification: Poster-2

Track Classification: Condensed Matter Physics