

Density Functional Theoretical Studies of the Photoelectron Spectroscopy with Carbon Fullerene materials

BY Dr. Himadri Chakraborty

Northwest Missouri State University

ABSTRACT

Quantized plasma waves in carbon valence electron clouds driven by photon or charged particle fields create plasmon resonances in the ionization of fullerene nanomaterials [1]. If the materials have composite structures, like nested fullerenes (buckyonions) or fullerenes endohedrally doped by an atom (endofullerenes), then plasmonic motions dynamically hybridize, leading to spectacular effects in the emission spectra [2, 3]. For fast ejected electrons, diffraction type modulations in the momentum space of emission intensities enrich the ionization process which offer an unusual spectroscopic route to image the charge cloud geometry [4, 5]. Using a time-dependent local density functional methodology we recently completed a number of studies of such processes for fullerene nanomaterials. Results have shown good agreements with available measurements. A selection of our findings will be discussed in the talk.

- [1] Madjet et al., *J. Phys. B* **41**, 105101 (2008)
- [2] McCune et al., *J. Phys. B Fast Track Comm.* **44**, 241002 (2011)
- [3] Madjet et al., *Phys. Rev. Lett.* **99**, 243003 (2007)
- [4] Patel et al., *J. Phys. B Fast Track Comm.* **44**, 191001 (2011)
- [5] Ruedel et al., *Phys. Rev. Lett.* **89**, 125503 (2002).

BIOGRAPHY

Presently, Himadri S. Chakraborty is an Associate Professor at Northwest Missouri State University in Maryville, Missouri. He has PhD from Georgia State University, Atlanta obtained in 1999. His research is focused on Computational Nanophysics, Materials Physics and AMO Physics. Before that, Himadri worked at Louisiana State University on the Attosecond Laser Pulse Generation and at J. R. MacDonald Lab, Kansas State University on ion-Surface Interactions. For two years, Himadri was Guest Scientist in Max-Planck-Institute for the Physics of Complex System in Dresden in Germany. His research is supported by NSF and DOE. Himadri was recognized as one of "50 Missourians You Should Know" in 2011.



EVENT DETAILS

DATE:

April 3, 2013

TIME:

11:00 AM

LOCATION:

Babbio 122
Stevens Institute of
Technology

ATTENDANCE:

Public

**Co-Sponsored by the
PEP Department**