Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Density functional studies of plasmons, hybridizations and electron diffractions in carbon fullerene nanomaterials[1] HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, USA, LAMINE MADJET, Center for Free Electron Laser Science, Hamburg, Germany — 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]. Further, 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, but smearing the ionic core into a jellium, we recently completed some studies of such processes for fullerene nanomaterials. Results have shown good agreements with measurements. [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).

[1]Supported by NSF, USA

Himadri Chakraborty
Northwest Missouri State University

Date submitted: 13 Nov 2012 Electronic form version 1.4