

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**High-resolution Valence and Core Excitation Spectra via First-Principles Calculations and Experiment**<sup>1</sup> ERIC SHIRLEY, NIST, F. FOS-SARD, ONERA-CNRS, LEM, K. GILMORE, ESRF, G. HUG, ONERA-CNRS, LEM, J.J. KAS, J.J. REHR, F. VILA, U. Wash., Seattle — We calculate the optical and C K-edge near edge spectra of crystalline and molecular C<sub>60</sub> measured with high-resolution electron energy-loss spectroscopy. The calculations are carried out using at least three different methods: Bethe-Salpeter calculations using the NIST Bethe-Salpeter Equation solver (NBSE) in the valence and OCEAN (Obtaining Core Excitation with Ab initio methods and NBSE) suite [Gilmore et al., *Comp. Phys. Comm.*, (2015)]; excited-core-hole calculations using XCH [D. Prendergast and G. Galli, *Phys. Rev. Lett.* 96, 215502 (2006)]; and constrained occupancy using StoBe (Stockholm-Berlin core-excitation code) [StoBe-deMon version 3.0, K. Hermann et al. (2009)]. They include self-energy effects, lifetime-damping, and Debye-Waller effects. A comparison of spectral features to those observed illustrates the sensitivity of certain features to computation details (e.g., self-energy corrections and core-hole screening). This may point to limitations of various approximations, e.g. in conventional BSE paradigm and/or the incomplete treatment of vibrational effects.

<sup>1</sup>Supported in part by DOE BES Grant DE-FG03-97ER45623 (JJR, JJK, FV)

Eric Shirley  
NIST

Date submitted: 03 Nov 2015

Electronic form version 1.4