A32.00003 : Ab initio modeling of STM elastic and inelastic tunneling spectra of tetramantane on Au(111) surface.
Authors: Emmanouil Kioupakis, R. Yamachika, Y. Wang, X.H. Lu, M.F. Crommie, Steven G. Louie
Monday, March 13, 8:24 AM–8:36 AM, Baltimore Convention Center – 329
Session A32: Fullerenes
Chair: Tunna Baruah, University of Texas, El Paso

A39.00007 : Electron phonon coupling and phonon renormalization in covalent metals
Authors: Peihong Zhang, Steven G. Louie, Marvin L. Cohen
Session A39: Focus Session: Magnesium Diboride and Related Compounds: Multi Gap Superconductivity
Chair: Lance Cooley, Brookhaven National Laboratory

G18.00001 : Excitons in the optical properties of nanotubes
Author: Catalin Spataru
Tuesday, March 14, 8:00 AM–8:12 AM, Baltimore Convention Center – 315
Session G18: Focus Session: Carbon Nanotubes: Electronic and Optical Properties I
Chair: Tobias Hertel, Vanderbilt University

G18.00004 : Diameter and chirality dependence of exciton properties in carbon nanotubes
Authors: Rodrigo Capaz, Catalin Spataru, Sohrab Ismail-Beigi, Steven Louie
Tuesday, March 14, 9:00 AM–9:12 AM, Baltimore Convention Center – 315
Session G18: Focus Session: Carbon Nanotubes: Electronic and Optical Properties I
Chair: Tobias Hertel, Vanderbilt University

K31.00005 : Accurate prediction of x-ray absorption spectra using density functional theory
Authors: David Prendergast, Giulia Galli
Tuesday, March 14, 3:42 PM–3:54 PM, Baltimore Convention Center - 328
Session K31: Focus Session: Simulation of Complex Materials III
Chair: Alberto Franceschetti, NREL

N18.00003 : Electrically Tunable Magnetic Properties of Defective Metallic Carbon Nanotubes
Authors: Young-Woo Son, Marvin L. Cohen, Steven G. Louie
Wednesday, March 15, 8:48 AM–9:00 AM, Baltimore Convention Center – 315
Session N18: Focus Session: Carbon Nanotubes: Transport I
Chair: Jun Kono, Rice University

N23.00010 : Ab initio calculations on the frustrated magnet ZnCr2O4
Authors: Kevin T. Chan, Jay D. Sau, Marvin L. Cohen, Peihong Zhang
Wednesday, March 15, 10:12 AM–10:24 AM, Baltimore Convention Center – 320
Session N23: Focus Session: MAG.THY III: Oxides and Phase Transitions
Chair: Bruce Harmon, Ames Laboratory

P10.00008 : First principles calculation of the x-ray absorption spectra of ice and liquid water
Authors: David Prendergast, Giulia Galli
Wednesday, March 15, 1:03 PM–1:15 PM, Baltimore Convention Center – 302
Session P10: Focus Session: Frontiers in Computational Chemical Physics IV
Chair: Andrew Rappe, University of Pennsylvania

P39.00012 : The role of the Fermi surface sampling in first-principles calculations of electron-phonon coupling
Authors: Feliciano Giustino, Marvin L. Cohen, Steven G. Louie
Wednesday, March 15, 1:51 PM–2:03 PM, Baltimore Convention Center - 342
Session P39: Focus Session: Supercconductivity-Theory and Computation (Mainly First Principles)
Chair: Ole Andersen, Max Planck Institute

R32.00004 : Dissipation of Mechanical Energy in Carbon Nanotube-based Mechanical Devices
Author: Paul Tanguay
Wednesday, March 15, 3:06 PM–3:18 PM, Baltimore Convention Center – 329
Session R32: Focus Session: Computational Nanoscience V
Chair: Wenchang Lu, NCSU

R37.00003 : Exploring the lead dependence of single-molecule conductance from first principles: The case of H2 molecular junctions
Authors: K.H. Khoo, J.B. Neaton, Steven G. Louie
Wednesday, March 15, 3:18 PM–3:30 PM, Baltimore Convention Center - 340
Session R37: Focus Session: Nanoscale Conductance Theory I
Chair: Mark Hybertsen, Columbia University

R37.00004 : Electronic level alignment at metal-molecule interfaces from first principles
Authors: Jeffrey B. Neaton, Mark S. Hybertsen, Steven G. Louie
Wednesday, March 15, 3:30 PM–3:42 PM, Baltimore Convention Center - 340
Session R37: Focus Session: Nanoscale Conductance Theory I
Chair: Mark Hybertsen, Columbia University

U6.00001 : LDA+U Based Studies of Electronic, Vibrational and Spectroscopic Properties of Solids
Author: Steven G. Louie
Thursday, March 16, 8:00 AM–8:12 AM, Baltimore Convention Center – 310
Session U6: Strong Electronic Correlation in Solids: Applications of the LDA+U method
Chair: Nicola Spaldin, UC Santa Barbara

U18.00007 : Electrical Switching in Metallic Carbon Nanotubes
Authors: Young-Woo Son, Hyoung Joon Choi, Jisoon Ihm, Marvin L. Cohen, Steven G. Louie
Thursday, March 16, 9:36 AM–9:48 AM, Baltimore Convention Center – 315
Session U18: Focus Session: Carbon Nanotubes: Transport III
Chair: Angel Rubio, DIPC San Sebastian

R37.00006 : Constrained LDA ab-initio calculation of screening of charging energy in C60
Authors: Jay Sau, Jeffrey Neaton, K.H. Khoo, Hyoung Joon Choi, Steven Louie, Marvin Cohen
Wednesday, March 15, 3:54 PM–4:06 PM, Baltimore Convention Center – 340
Session R37: Focus Session: Nanoscale Conductance Theory I
Chair: Mark Hybertsen, Columbia University

V36.00003 : First-Principles study of the optical properties of BN nanotubes and h-BN
Authors: Cheol Hwan Park, Catalin Spataru, Steven Louie
Thursday, March 16, 12:03 PM–12:15 PM, Baltimore Convention Center – 339
Session V36: Focus Session: Optical Properties of Carbon Nanotubes and C60
Chair: Eric Shirley, NIST

V36.00005 : Bound excitons and optical absorption spectra of (10,10) metallic single-walled carbon nanotubes
Authors: Jack Deslippe, Catalin Spataru, Steven Louie
Thursday, March 16, 12:27 PM–12:39 PM, Baltimore Convention Center – 339
Session V36: Focus Session: Optical Properties of Carbon Nanotubes and C60
Chair: Eric Shirley, NIST

V38.00009 : Stability Constraints and Local Criteria for the Bounds on Te of Conventional Superconductors
Authors: Jonathan E. Moussa, Marvin L. Cohen
Thursday, March 16, 12:51 PM–1:03 PM, Baltimore Convention Center – 341
Session V38: Superconductivity-Thermodynamics and Structure
Chair: Jeff Tallon, Industrial Research Limited

Z37.00001 : First-principles studies of the electronic structure of cyclopentene on Si(100)
Authors: Su Ying Quek, Jeffrey Neaton, Mark Hybertsen, Effthimos Kaxiras, Steven Louie
Friday, March 17, 11:15 AM–11:27 AM, Baltimore Convention Center - 340
Session Z37: Focus Session: Nanoscale Conductance Theory III
Chair: Jeffrey Neaton, (LBNL)