

Poster Session I
Saturday, March 21, 2009

- PI-1 Sabrina S. Carara, Ronaldo J.C. Batista, and Helio Chacham
"Modifications in Graphene's Electron States Due to a Deposited Lattice of Au Nanoparticles"
- PI-2 Vincent Crespi
"Geometrical Constraints in Nanochemical Physics"
- PI-3 Jack Deslippe, David G. Prendergast, and Steven G. Louie
"Electronic and Optical Properties of Nanostructures"
- PI-4 Guang-Yu Guo, Hung-Chung Hsueh, and Steven G. Louie
"Excitonic Effects and Optical Spectra of Nitride Semiconductors and Their Nanowires"
- PI-5 Sohrab Ismail-Beigi
"New Exact And Approximate Forms for the Luttinger-Ward Correlation Energy Functional Within The GW-RPA Approximation"
- PI-6 Koichiro Kato and Susumu Saito
"Work Function of Carbon Nanotubes"
- PI-7 Hoonkyung Lee, Jisoon Ihm, Marvin L. Cohen, and Steven G. Louie
"Calcium-Decorated Carbon Nanotubes for High-Capacity Hydrogen Storage"
- PI-8 Andre A. Lino, Helio Chacham, and Mario S. C. Mazzoni
"Electronic States in TiO₂ Nanoribbons"
- PI-9 Yoshiyuki Miyamoto
"Electron-Ion Dynamics in Condensed Matters Under Strong Optical Field"
- PI-10 Jonathan E. Moussa
"Brief Introduction to the Truncated Eigenfermion Decomposition"
- PI-11 Tadashi Ogitsu
"A Frustrated Elemental Solid: β -Rhombohedral Boron"

- PI-12 Su Ying Quek, Hyoung Joon Choi, Steven G. Louie, Mark S. Hybertsen, Latha Venkataraman, and Jeffrey B. Neaton
“Theoretical Studies of the Conductance of Single Molecule Junctions”
- PI-13 Steven L. Richardson, Rajendra. R. Zope, Tunna Baruah, and Mark R. Pederson
“First-Principles Studies of the Electronic and Vibrational Properties of Hexagonal Diamondoids”
- PI-14 Ivo Souza
“Orientation Dependence of the Anomalous Hall Effect in hcp Cobalt”
- PI-15 Steven Whitelam
“Transformation from Spots to Waves in a Model of Actin Pattern Formation”
- PI-16 Li Yang, Jack Deslippe, Cheol-Hwan Park, Marvin L. Cohen, and Steven G. Louie
“Many-Electron Effects on the Electronic Structure and Optical Spectrum of Few-Layer Graphene”
- PI-17 Shenyuan Yang, David G. Prendergast, and Jeffrey B. Neaton
“First-Principles Studies of Structure and Electronic Level Alignment at CdSe/CdTe Heterojunctions”
- PI-18 Yu Xue and Peihong Zhang
“First-Principles Theory of Coloration of WO₃ Upon Charge Insertion”

Poster Session II
Sunday, March 22, 2009

- PII-1 L. Chico, H.Santos M. Pelc, W. Jaskólski, and A. Ayuela
“Friedel-like oscillations in carbon nanotube quantum dots and superlattices”
- PII-2 T. H. Cho, W. S. Su, T. C. Lueng, Wei Ren , and C. T. Chan
“Electronic and Optical Properties of Single-Walled Carbon Nanotubes Under External Electric Field: A First Principles Study”
- PII-3 Michel Côte
“Electron-Phonon Coupling in C₆₀ Using Hybrid Functionals”
- PII-4 Hung-Chung Hsueh, Guang-Yu Guo, and Steven G. Louie
“Quasiparticle and Excitonic Effects in the Optical Properties of SiC Nanotubes”
- PII-5 Leeor Kronik
“Reliable Prediction of Charge Transfer Excitations in Molecular Complexes Using Time-Dependent Density Functional Theory”
- PII-6 Weidong Luo and Sokrates T. Pantelides
“Charge Ordering, Orbital Occupancy, and Electron Spectroscopy of Manganites”
- PII-7 Kaoru Ohno, Soh Ishii, Yoichi Tadokoro, and Yoshifumi Noguchi
“All-Electron Mixed-Basis Approach For The Excited States Of Materials”
- PII-8 Young-Woo Son, Li Yang, Cheol-Hwan Park, Marvin L. Cohen, and Steven G. Louie
“Physics of Graphene, Nanoribbons, and Superlattices”
- PII-9 David Prendergast
“The Shirley Interpolation Suite”
- PII-10 Masahiro Sakurai and Susumu Saito
“Constant-Pressure MD Simulation for Small-Diameter Single-Walled Carbon Nanotubes”
- PII-11 David A. Strubbe, Xavier Andrade, Angel Rubio, and Steven G. Louie
“Non-Linear Optics And Local-Field Factors In Liquid Chloroform: A Time-Dependent Density-Functional Theory Study”

- PII-12 Brandon C. Wood
“Degradation of semiconductor photoelectrodes in aqueous environments from ab-initio molecular dynamics”
- PII-13 Alexey T. Zayak and Jeffrey B. Neaton
“First-Principles Studies Of Surface-Enhanced Raman Scattering: Benzene Thiol On Au (111)”
- PII-14 Yiyang Sun, Yong-Hyun Kim, Kyuho Lee, Damien West, and S. B. Zhang
“Spin Control by Molecular Hydrogen Adsorption in Metal-Organic Frameworks”