Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Optical and Magnetic Properties of WS$_2$: Single Layers, Clusters, and Nanoribbons

FLORENTINO LOPEZ-URIAS, Advanced Materials Department, IPICYT, Camino a Presa San Jose 2055, Col. Lomas 4a Sección, San Luis Potosí, México, HUMBERTO R. GUTIERREZ, Department of Physics and Astronomy, University of Louisville, Louisville, KY 40292 USA., NESTOR PEREA-LOPEZ, ANA LAURA ELIAS, AYSE BERKDEMIR, Department of Physics, The Pennsylvania State University, University Park, PA 16802, USA, ANDRES CASTRO-BELTRAN, Facultad de ingeniera Mecanica y Electrica, Universidad Autonoma de Nuevo Leon, Avenida Universidad s/n Ciudad Universitaria, C.P.66450, San Nicolas, RUITAO RU, HUMBERTO TERRONES, Department of Physics, The Pennsylvania State University, University Park, PA 16802, USA, MAURICIO TERRONES, Pennsylvania State University and Research Center for Exotic Nanocarbons (JST), Shinshu University, Wakasato 4-17-1, Nagano 380-8553, Japan — Transition metal chalcogenides are layered materials, similar to graphite. Inspired in recent experiments on the synthesis and photoluminescence enhancement of single-layer WS$_2$ sheets and triangular islands, in the present work, first-principles density functional theory calculations are carried out on different WS$_2$ nanostructures. In addition, we have studied WS$_2$ clusters with different 2-D morphologies, nanoribbons with zigzag and armchair edges, as well as single- and few-layered WS$_2$. The electronic density of states, scanning tunneling microscopy simulations, structural and magnetic ordering stability, and edge chirality are studied. Bethe-Salpeter equation for the electron-hole two particle Green function has been solved in order to calculate the in-plane polarized optical spectrum and exciton wave functions. In addition, the role of spin-orbit coupling on the electronic properties of single layer WS$_2$ is discussed.

Florentino Lopez-Urias
Advanced Materials Department, IPICYT,
Camino a Presa San Jose 2055,
Col. Lomas 4a Sección, San Luis Potosí, México

Date submitted: 20 Dec 2012