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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 photoluminesce 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.

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