

Abstract Submitted  
for the MAS14 Meeting of  
The American Physical Society

**Electronic properties of rhenium doped tungsten disulfide monolayers** EDUARDO CRUZ-SILVA, AMBER MCCREARY, NESTOR PEREA-LOPEZ, ANA LAURA ELIAS, Department of Physics and Center for 2-Dimensional and Layered Materials, The Pennsylvania State University, HUMBERTO TERRONES, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, MAURICIO TERRONES, Department of Physics and Center for 2-Dimensional and Layered Materials, The Pennsylvania State University — Layered transition metal dichalcogenides (TMDs) have attracted attention due to their electronic and optical properties. In particular, MoS<sub>2</sub> and WS<sub>2</sub> show an indirect to direct electronic band gap transition when reduced to a monolayer, and display strong photoluminescence. While there are proposed applications for MoS<sub>2</sub> and WS<sub>2</sub> as electronic and optoelectronic devices, control of their electronic properties needs to be reached before these applications can be scaled. Chemical doping has been recently shown to allow the modification of the electronic properties of MoS<sub>2</sub> monolayers by substitution of either transition metals or the chalcogen. Here we present an experimental and computational study of the electronic and optical properties of doped WS<sub>2</sub> monolayers. Re-doped WS<sub>2</sub> monolayers have been produced by chemical vapor deposition (CVD). Photoluminescence and Raman spectroscopy studies suggest that rhenium atoms have been successfully incorporated into WS<sub>2</sub> lattice. *Ab initio* calculations indicate that substitution of W atoms by Re results in the formation of new states in the vicinity of the Fermi energy that allows tailoring of the electronic band gaps, which also results in different optical properties.

Eduardo Cruz-Silva  
Dept of Physics and Center for 2-Dimensional and Layered Materials,  
The Pennsylvania State University

Date submitted: 29 Aug 2014

Electronic form version 1.4