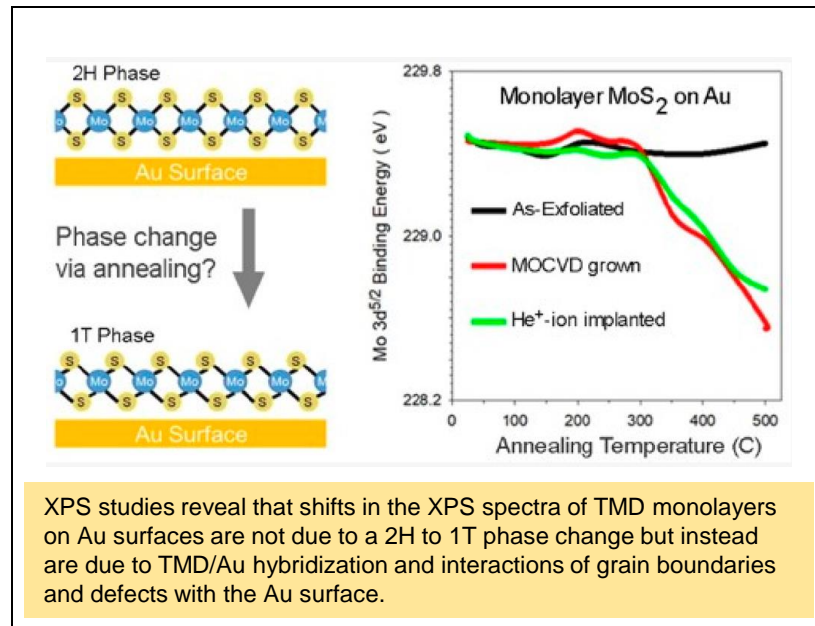


G.G. Jernigan, J.J. Fonseca, C.D. Cress and J.T. Robinson (NRL)  
T.H. Choudhury and M. Chubarov (2DCC-MIP)

**Project Summary:** The electronic properties of transition metal dichalcogenides (TMDs) vary dramatically depending on their phase (2H vs. 1T) and the energy to convert between the two phases is predicted to be relatively low. This has sparked interest in the use of the phase change properties of TMDs for active components in electronic devices. A combination of mechanical strain and charge transfer from a metal substrate has previously been suggested to induce the phase transition from 2H to 1T. In this study, x-ray and ultraviolet photoelectron spectroscopy (XPS, UPS) were used to identify charge transfer processes and changes in the structural phase for MoS<sub>2</sub>, MoSe<sub>2</sub> and MoTe<sub>2</sub> monolayers on Au surfaces annealed up to 500°C. Although charge transfer does appear to occur, we do not find spectroscopic evidence for the 2H to 1T phase change in exfoliated TMDs. However, both helium-ion irradiated exfoliated TMDs and layers grown by metalorganic chemical vapor deposition (MOCVD) show shifts in their XPS spectra that could be interpreted as a phase change but instead are the result of TMD/Au hybridization, grain boundaries and defects interacting with the Au surface.

Published in: *J. Phys. Chem. 2020, 124, 25361-25368.*

**2DCC Role:** The wafer-scale MoS<sub>2</sub> monolayer samples used for this study were grown by MOCVD in the 2DCC facility. The user PI (J.T. Robinson) and his postdoctoral scholars have been active participants in 2DCC activities including participating in annual User Committee meetings and presenting posters at Graphene and Beyond.



XPS studies reveal that shifts in the XPS spectra of TMD monolayers on Au surfaces are not due to a 2H to 1T phase change but instead are due to TMD/Au hybridization and interactions of grain boundaries and defects with the Au surface.