

Materials Chemistry Seminar

**Friday, March 22, 2024
11:30 a.m. ~ BRWN 4102**

"Effect of Annealing on Tunable Electronic Properties of Metal Intercalated WS₂"



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Abstract:

High carrier mobility and chemical stability in semi-conducting two-dimensional metal dichalcogenides (TMDs) is required to integrate them into nanoscale flexible devices. Previously, our group developed a solution-based synthesis method to intercalate transition metal ions into 1T'-Li_xWS₂. The hybridization of the 3d orbitals of the transition metal intercalant with the conduction band of WS₂ enabled high conductivity and improved carrier mobility in the semi-metallic 1T' phase of WS₂. In this work, we use a thermal annealing strategy to transform the as-synthesized TM-intercalated WS₂ from the 1T' phase to the semiconducting 2H phase. By varying the annealing temperature and heating rate, we observe systematic changes in the degree of phase transformation from 1T' to 2H, metal intercalant retention, and interlayer compression based on powder XRD and Raman mapping data. DRUV-Vis shows that the band gap of vanadium-intercalated WS₂ after annealing at 400°C is 1.56eV, 180 meV lower than pristine 2H-WS₂. We also observed a change in the conductivity and carrier activation energy of this phase-transformed material compared to bulk WS₂ and 1T'-V-intercalated WS₂. Future work will be focused on characterizing the distribution and homogeneity of the V dopant in the annealed WS₂ sheets to understand its role in electronic structure.

Bio:

Mah Gull is a second-year grad student in Professor Christina Li's group. She did her BS from the University of Punjab and MS from the Lahore University of Management Sciences, Pakistan where she worked under Dr. Muhammad Zaheer on Single-Site Heterogeneous Catalysts Based on Bimetallic Metal-Organic Frameworks (MOFs). She joined the Li Lab in Fall 2023. Currently, she is working on Effect of Annealing on Tunable Electronic Properties of Metal Intercalated WS₂. In her free time, she likes to spend time with friends, cooking, or watch K- Dramas.