Tuneable Structural and Optoelectronic Properties of Doped and Undoped Ternary 2-D Transition Metal Dichalcogenides for Photovoltaic Applications

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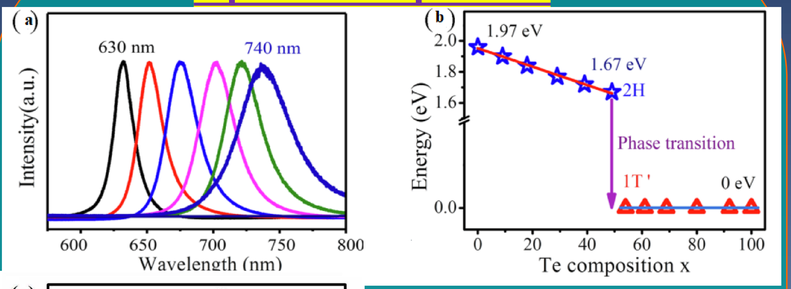
Introduction

- Ternary TMDs are capable of stoichiometric variation, band gap tuning and phase transitions.
- Most TMDs are underexplored and there exists much opportunity for research in this field.

Optical Properties

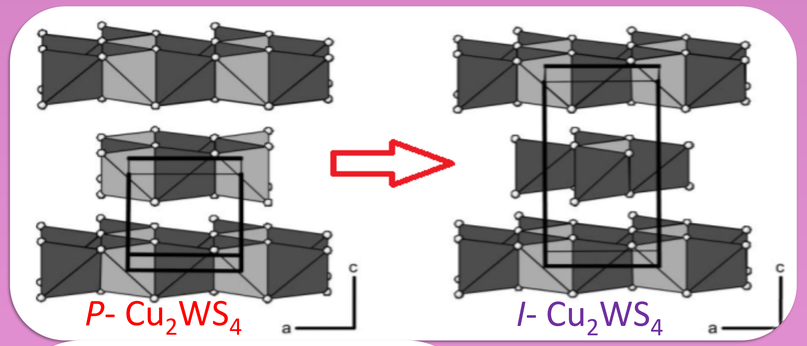


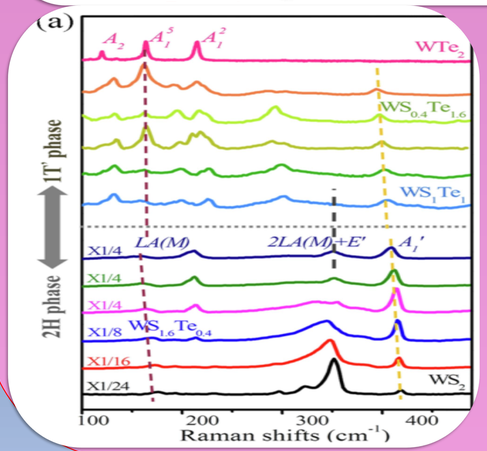
- A- Te composition dependent PL spectrum of monolayer 2H phase $WS_{2(1-x)}Te_{2x}$ alloys.
- B- Optical bandgap values of 2H and 1T' phase $WS_{2(1-x)}Te_{2x}$ alloys.
- C- Absorption spectrum and Tauc plot of CWS (1.8eV) matches well with the solar spectrum.
- Suitable candidates for photovoltaic applications.

Structural Tuneability

P- Cu_2WS_4 to *I*-Cu_2WS_4 Transition

- Low Temperature and Low Pressure: *P*- Cu_2WS_4
- High Temperatures and High Pressure: *I*-Cu_2WS_4
- Colloidal Synthesis : *I*-Cu_2WS_4





2H to IT' Polytype Transition

Changing composition of X in $WS_{2(1-x)}Te_{2x}$ alloy system.

Our Protocol

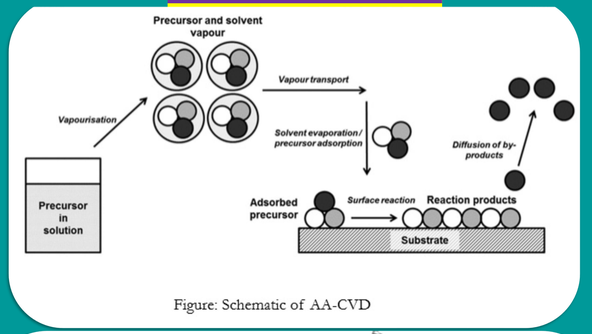
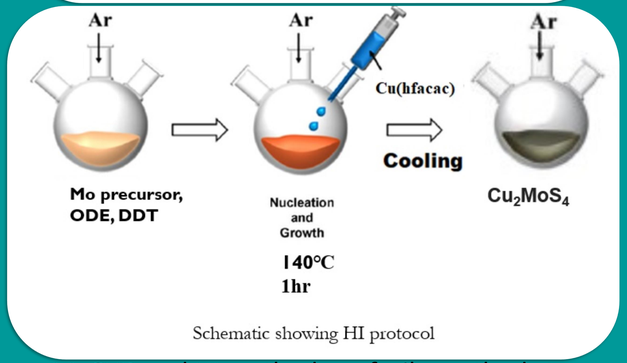


Figure: Schematic of AA-CVD



Schematic showing HI protocol

- AA-CVD and HI method are facile methods to introduce and control dopants into ternary systems.
- Investigation of diethyldithiocarbamates and xanthates as precursors.
- Manipulation of reaction parameters.
- Obtain favourable structural diversity and optoelectronic properties.

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2. Gulen, M.; Sarilmaz, A.; Patir, I. H.; Ozel, F.; Sonmezoglu, S. Ternary Copper-Tungsten-Disulfide Nanocube Inks as Catalyst for Highly Efficient Dye-Sensitized Solar Cells. *Electrochimica Acta* **2018**, *269*, 119–127.
3. Wang, Z.; Sun, J.; Wang, H.; Lei, Y.; Xie, Y.; Wang, G.; Zhao, Y.; Li, X.; Xu, H.; Yang, X.; Feng, L.; Ma, X. 2H/1T' Phase WS2(1−x)Te2x Alloys Grown by Chemical Vapor DEPOSITION with Tunable Band Structures. *Applied Surface Science* **2020**, *504*, 144371.