

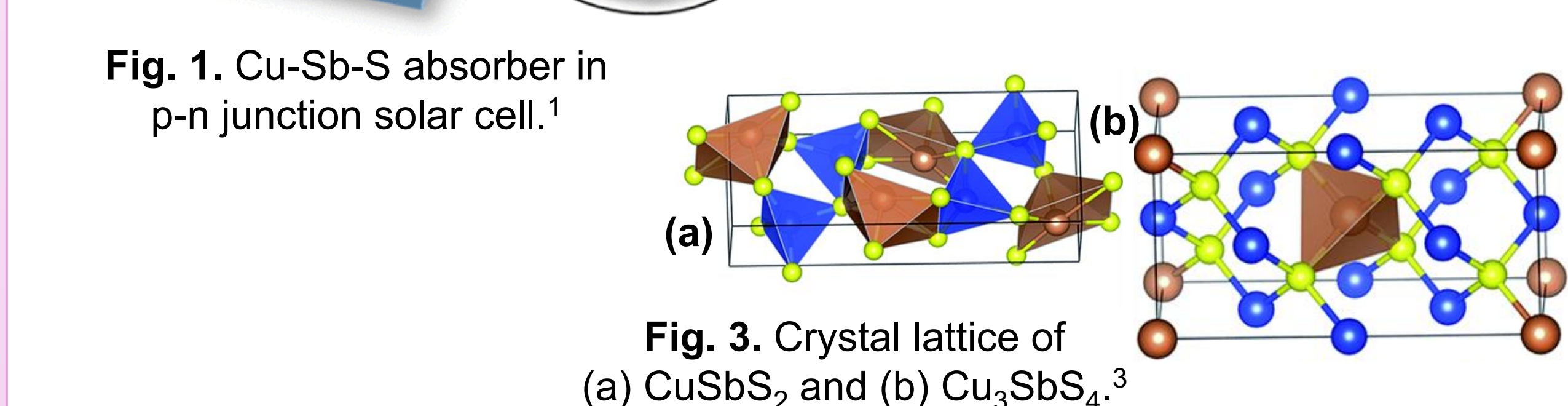
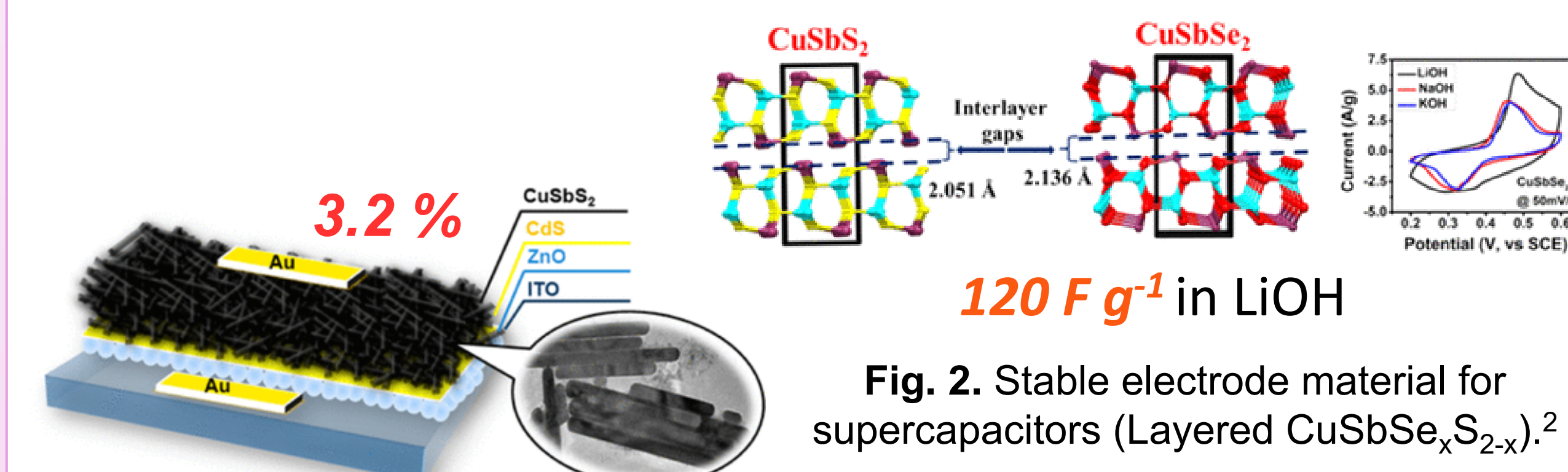
Tuning Structure and Function: Metal-Ion Induced Phase Transformation in Copper Antimony Sulphide Nanosheets

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Introduction

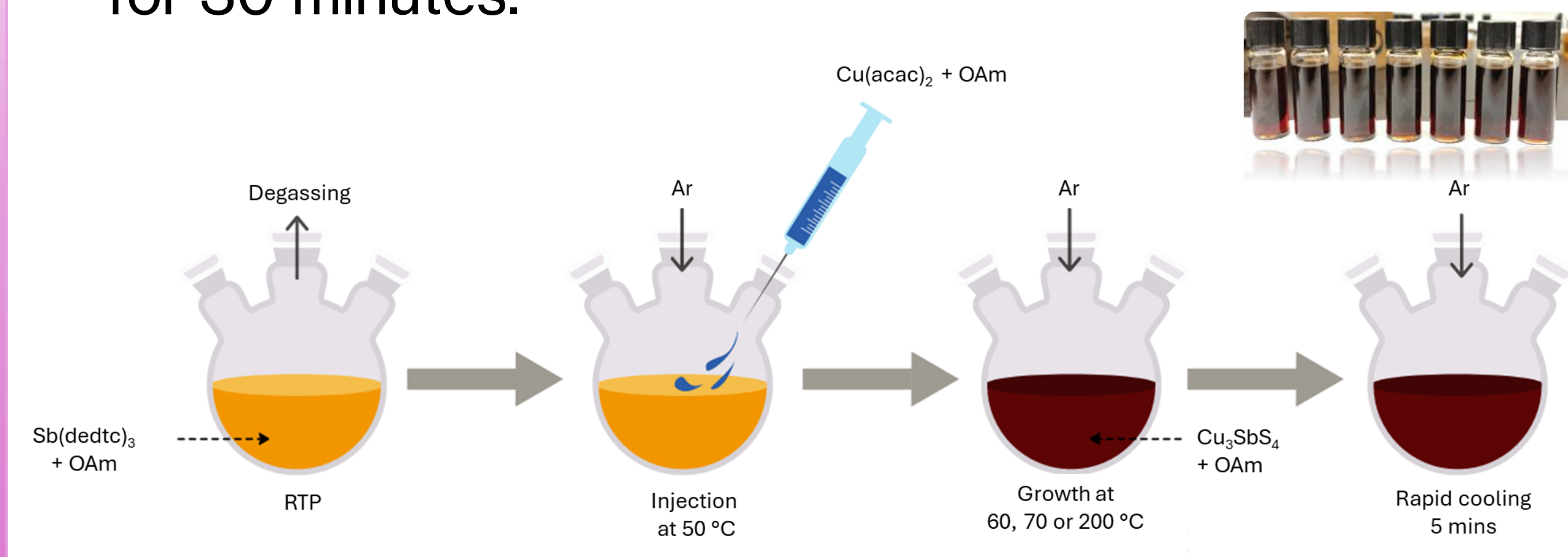
Cu-Sb-S for photovoltaics/energy storage since it has:

- Structure, composition, and stoichiometry versatility
- Excellent, broad variation of intrinsic functional properties
- Earth abundance, low cost, environmental and benign health effects
- Tunable optical & electrochemical properties



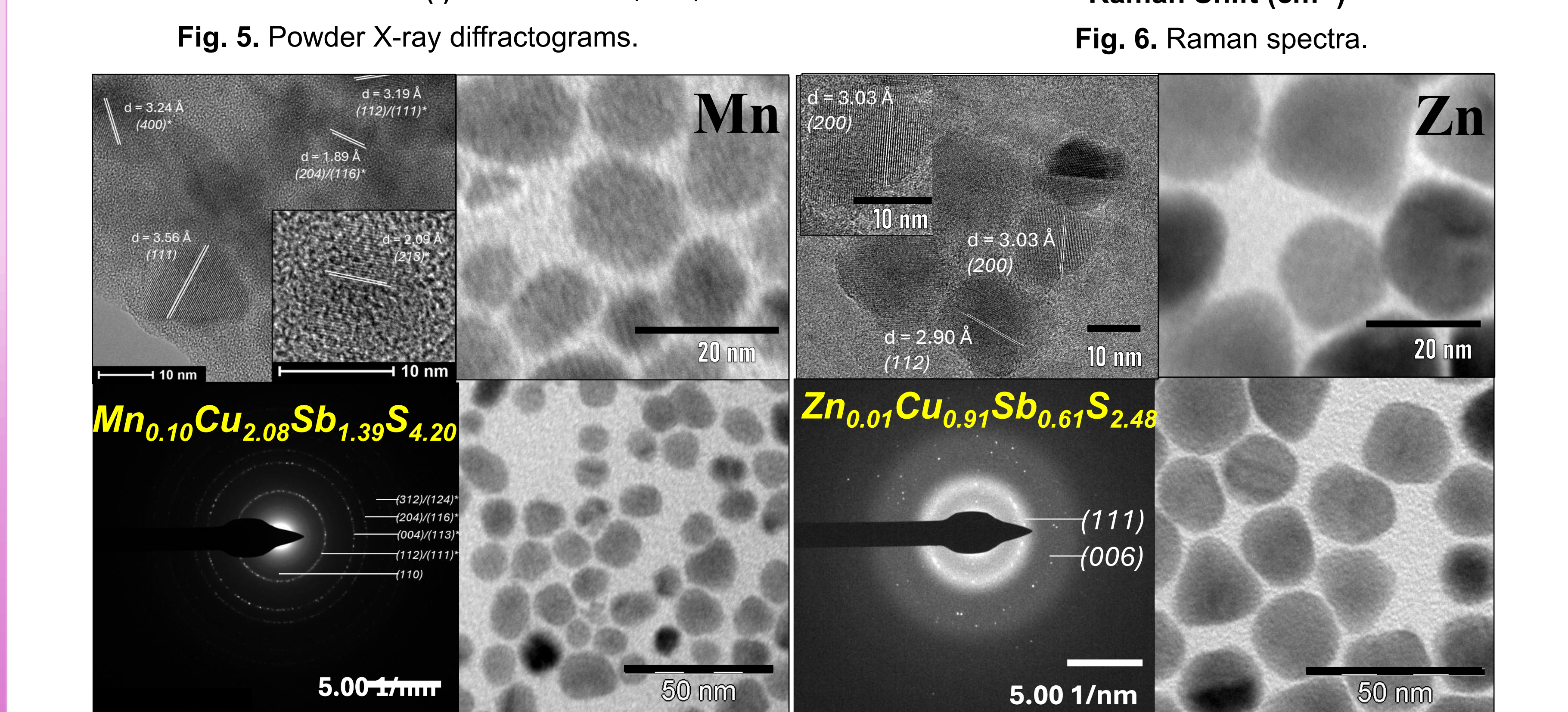
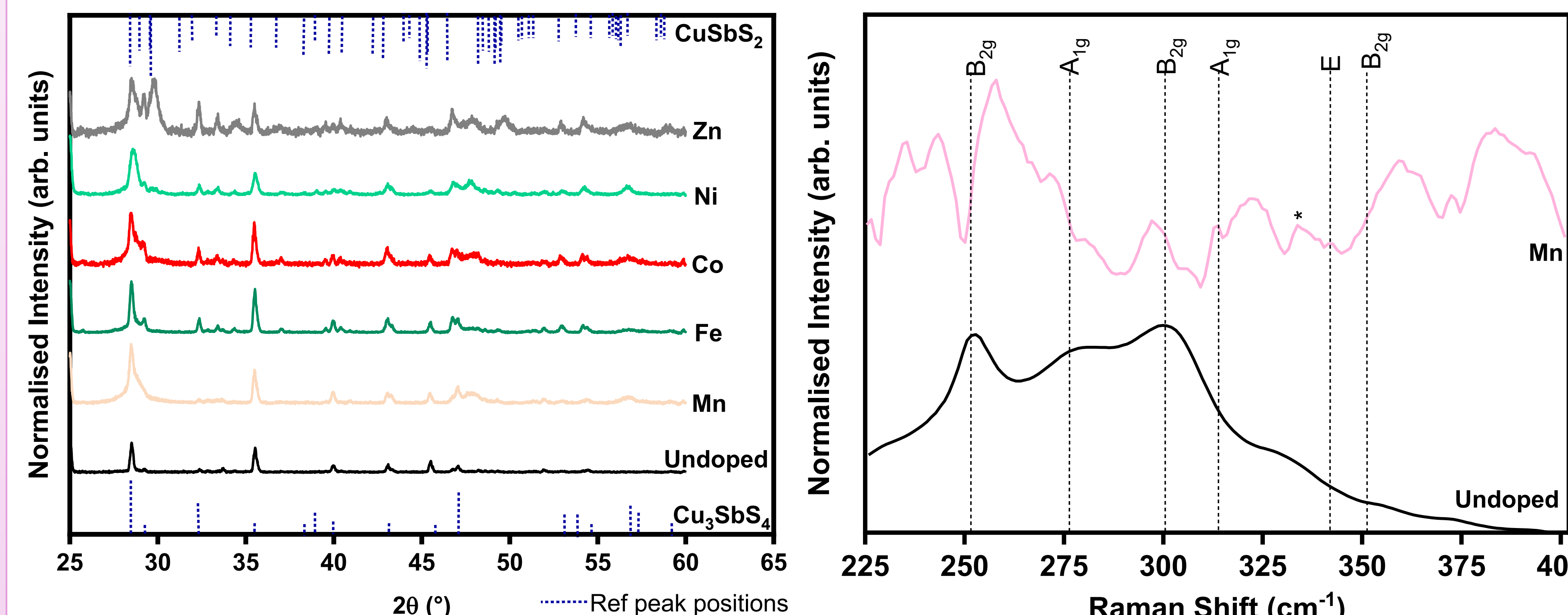
Colloidal (Hot-Injection) Synthesis

- Injection of Cu(acac)₂ + sulfonated OAm (Oleylamine) solution into a reaction flask containing Sb(ddtc)₃ + OAm solution held at 50 °C. The mixture was quickly ramped to 200 °C and NPs were grown for 30 minutes.



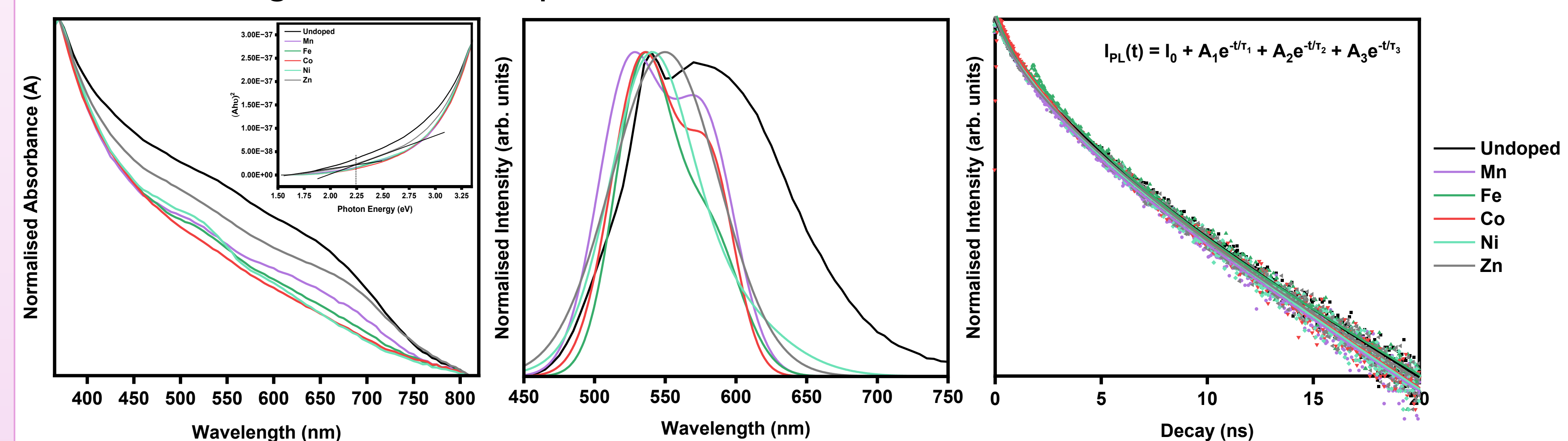
Metal ion-induced fCAS to cCAS Phase Transformation

- p-XRD data confirm a novel phase transformation from a **tetragonal** structure to an **orthorhombic** one with heavier metal ion dopant.
- Representative Raman spectroscopy data reveal a **mixed phase system**.
- HR-S/TEM and SAED data corroborate with p-XRD data and confirm the **tetragonal** and **orthorhombic** structures of doped CAS NPs.
- TEM and EDS suggest a correlation of morphology and composition of NPs with dopant ion.



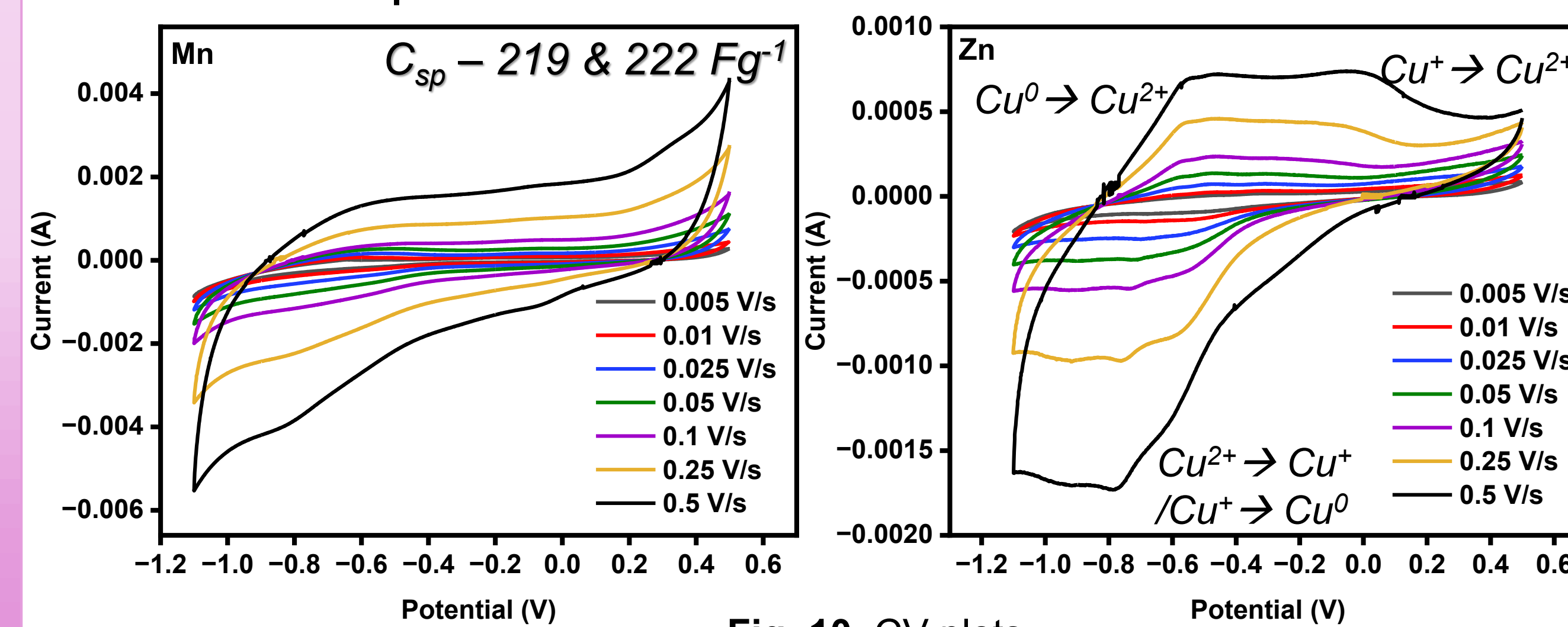
Dopant-Induced Photophysical Variation

- Doped NPs:
 - bandgaps decrease from **2.58 eV** (undoped) to range between **2.17 to 2.38 eV**.
 - show blueshifted emission (~537 nm) with narrower FWHM.
 - have lengthened fast triple radiative recombination.



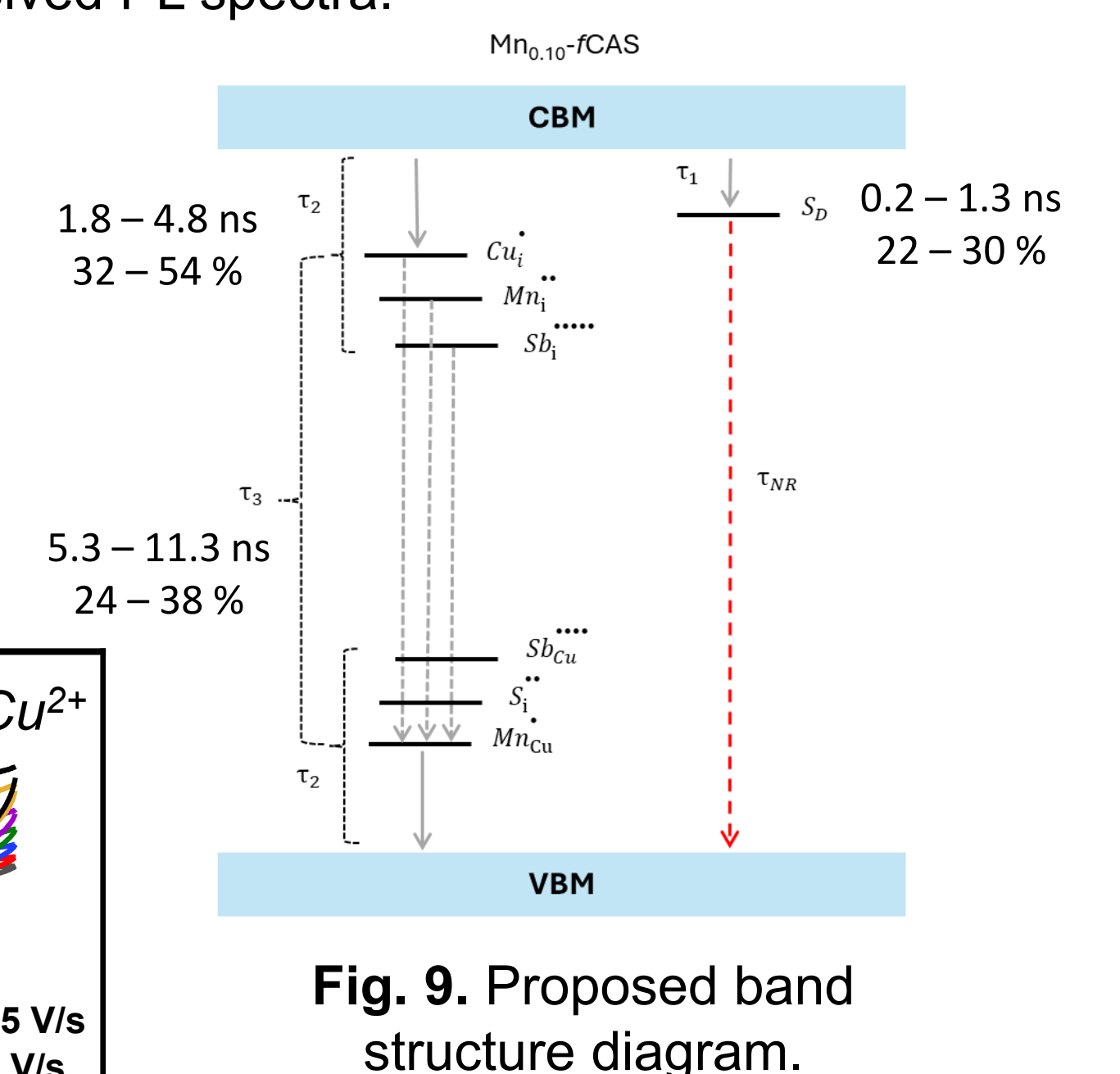
Phase-dependent Pseudocapacitance

- Metal ion doping - especially with Zn²⁺ - enhances pseudocapacitance through a phase transition to chalcostibite, improving redox activity, conductivity, and ion transport.



Conclusions

- Metal-ion induced phase transformation results in bandgap tunability (narrowed) and enhanced pseudocapacitance (almost 3-fold).



References

1. Suehiro, S.; et. al; *Inorganic Chemistry* **2015**, 54 (16), 7840-7845.
2. Ramasamy, K.; et. al; *Chemistry Materials* **2015**, 27 (1), 379-386.
3. Zakutayev, A.; et. al; Conference Paper, 2014.