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From TMDCs to Ternary Chalcogenides: Material-Specific Pathways to 2D Sulvanite Nanostructures

Daniela R. Radu, Florida International University

Presentation Abstract

2D sulvanites (Cu_3MX_4; M = V, Nb, Ta; X = S, Se, Te) are an emerging class of ternary copper chalcogenides with promising optical and electronic properties. These compounds crystallize in a cubic structure with tetrahedral coordination between the metal center and surrounding chalcogen atoms. While traditional colloidal syntheses of sulvanites rely on hot-injection techniques and typically yield cuboid morphologies, we report a solution-phase approach that enables the formation of 2D sulvanite nanosheets through a sequential precursor injection strategy. Specifically, when targeting Cu_3VS_4 and Cu_3VSe_4, we observed that adding vanadium precursors to sulfur or selenium solutions leads to the initial formation of VS_2 or VSe_2 nanosheets, respectively. Upon subsequent copper incorporation, these precursors transform into the corresponding sulvanite compounds while preserving the 2D sheet morphology, diverging from the commonly reported cuboid structures. This reaction pathway suggests a morphology-retentive conversion mechanism, possibly governed by topotactic transformation from TMDC intermediates. However, applying the same strategy to $NbSe_2$ led instead to the formation of Cu_3NbSe_4 with a cuboid morphology, indicating a material-specific response to copper introduction. These observations highlight nuanced differences in reactivity and structural adaptability across transition metal systems, emphasizing the need to understand precursor chemistry and reaction dynamics in morphology-controlled synthesis. This work provides new insight into solution-based approaches for fabricating 2D sulvanites and opens opportunities to design novel nanostructures for optoelectronic and energy applications.