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SEMICONDUCTING LAYERED TRANSITION-METAL DICHALCOGENIDES: INSIGHTS FROM FIRST-PRINCIPLES

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Transition-metal dichalcogenides (TMDCs) are an important class of inorganic materials exhibiting a wide spectrum of catalytic, electronic, magnetic, and optical properties [1]. In particular, TMDCs with layered structures such as MoS_2 are considered attractive for use in next-generation nanoscale flexible field-effect transistor (FETs) devices [2] and for the important areas of industrial heterogeneous catalysis [3]. TMDCs nanomaterials (i.e., nanotubes and fullerene- or onion-like structures) have also emerged as possible applications as photodetectors or photo electrochemical solar cells [4].

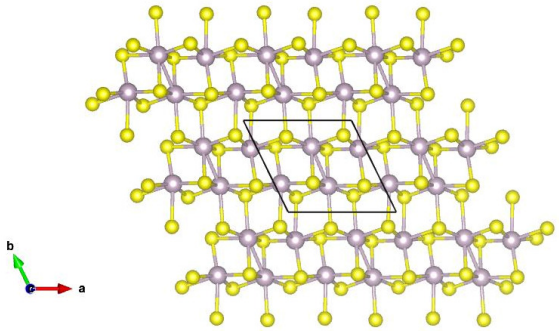

Figure 1. Ball-and-stick model of the layered TcX_2 (X=S and Se). Top view along the normal to the (a,b) plane. Color legend: Tc, blue; X, yellow.

Among TMDCs, relatively limited knowledge is available on technetium dichalcogenides (**Figure 1**). A systematic study of the structures and properties of layered technetium dichalcogenides investigated using density functional theory (DFT) [5] indicates that they are semiconducting. Structure-property relationships of this fascinating tunable bandgap materials will be discussed in this talk.

References

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