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First principles study of the 2D Mo(S1-XTeX)$_2$ TMD alloy: in bulk; Adsorbed on an Al-terminated Sapphire; Between Layers of Graphene; on Graphite; and on GaN

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First principles based computational studies were performed for dichalcogenide alloys, mostly Mo(S,Te)$_2$, in bulk, adsorbed on Al-terminated sapphire, on graphite, and on GaN, and sandwiched between two layers of graphene. In bulk, predicted phase relations for Mo(S,Te)$_2$ and W(S,Te)$_2$ are dominated by phase separation, but when the Mo(S,Te)$_2$ alloy is in contact with sapphire, graphite, graphene, or GaN predicted phase relations are dominated by S:Te-ordering. The results of First Principles Phase Diagram (FPPD) calculations, binding energy calculations, and predicted band-gap variations, as functions of bulk composition, will be presented.