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Density functional theory study of the role of the alkali and chalcogen atoms on the stability of quaternary chalcogenides $A_2M^{II}M_3^{IV}Q_8$

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Layered chalcogenide compounds are good candidates to obtain two-dimensional materials, which have attracted great attention for potential technological applications and advances in basic science . Because of the structural diversity among chalcogenides, a good description of the factors that influence the stability of layered structures is desired, specially for complex compositions, such as ternary and quaternary materials. (1) To improve the atomistic understanding of the major roles that affect the formation of layered quaternary chalcogenides, we performed density functional theory calculations with van der Waals corrections for the $A_2ZnSn_3Q_8$ materials (A = Li, K, Cs; Q = S, Se, Te), employing three experimental layered and three-dimensional crystal structures. The calculations yield equilibrium lattice parameters that are in good agreement with experimental data, and therefore provide a good description of the structural properties. (2) Our results show that the atomic radii of the alkali metal and chalcogen species play an important role in the stability of the structures. The layered structures are favored for compositions in which the average of the atomic radii of A and Q are in the regions of smaller or larger values, while the closed three-dimensional structures are the most energetically stable in the intermediate region. These results can be explained based on the minimization of strain, that tends to favor the less compact structures for larger atoms, and its interplay with the coulomb repulsion of the anionic framework. This understanding can help to guide the search for layered quaternary chalcogenide materials.

Keywords: Chalcogenides. Layered materials. Density functional theory.

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2 BESSE, R.; DA SILVA, J. L. F. The role of the alkali and chalcogen atoms on the stability of the layered chalcogenide $A_2M^{II}M_3^{IV}Q_8$ (A = alkali-metal; Q = chalcogen) compounds:. a density functional theory investigation within van der Waals corrections. **Journal of Physics**: condensed matter. Submitted.