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Two-dimensional group-IV monochalcogenides: structural, electronic and optical properties.[1] LIDIA GOMES, ALEXANDRA CARVALHO, A. H. CASTRO NETO, National University of Singapore — Two-dimensional materials have attracted a massive attention of the scientific and industrial communities due to their unusual and interesting properties. The layered group-IV monochalcogenides-SnS, SnSe, GeS and GeSe- has gained attention as a promising group with potentially useful applications in diverse fields. The bulk SnS, a naturally occurring mineral, has been considered as an alternative to be used in film PV cells, due to its electronic and optical properties. We use first principles calculations to explore structural, electronic and optical properties of this group, with focus in their two-dimensional forms. We show that all those binary compounds are semiconducting, with bandgap energies covering most of the visible range. They have multiple valleys in the valence and conduction bands, with spin-orbit splitting of the order of 19-86 meV. An enhanced static dielectric permittivity is found for the monolayers. Structural analysis shows that the 2D form of these materials presents very high piezoelectric constants, exceeding values recently observed for other 2D-systems. The existence of a negative Poisson ratio is predicted for the GeS compound.

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