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An Array of Layers in Silicon Sulfides: Chain-like and Ground State Structures¹ TOMÁS ALONSO-LANZA, ANDRÉS AYUELA, (CSIC-UPV/EHU), Materials Physics Center (MPC), Donostia Int. Physics Center (DIPC, FAUSTINO AGUILERA-GRANJA, Universidad Autónoma de San Luis de Potosí, México — While much is known about isoelectronic materials related to carbon nanostructures, such as boron nitride layers and nanotubes, rather less is known about equivalent silicon based materials. Following the recent discovery of phosphorene, we here discuss isoelectronic silicon monosulfide monolayers. We describe a set of anisotropic ground state structures that clearly have a high stability with respect to the near isotropic silicon monosulfide monolayers. The source of the layer anisotropy is related to the presence of Si-S double chains linked by some Si-Si covalent bonds, which lie at the core of the increased stability, together with a remarkable *spd* hybridization on Si. The involvement of *d* orbitals brings more variety to silicon-sulfide based nanostructures that are isoelectronic to phosphorene, which could be relevant for future applications, adding extra degrees of freedom.

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