

# Elemental two-dimensional materials : Novel electronic and structural properties

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We present our recent studies on the thermodynamical stability, mechanical, electronic, structural and optoelectronic properties of elemental 2D materials (Si, Ge, Sn, Se and Te). We predicted new single and multi-layered-phases of silicon which exhibit strong directionality in the electronic and structural properties. They have wider indirect band gaps but also increased absorption in the visible range making them more interesting for photovoltaic applications. Moreover, the intrinsic two-dimensional confinement and strong electron-phonon coupling make them a candidate material for thermoelectricity and superconductivity. We have identified a novel stable 2D layered structure for group VI elements Se and Te that we call square selenene and square tellurene, respectively. They have chair-like buckled structures similar to other 2D such as silicene and germanene but with a square unit cell. This special structure gives rise to anisotropic band dispersions near the Fermi level. The large band gap (0.1 eV) opened by spin-orbit coupling makes Se and Te topological insulators, hosting non-trivial edge states. They are promising materials for electronic/spintronics applications.