Quasi-2D silicon structures based on ultrathin Me2Si (Me = Mg, Ca, Sr, Ba) films

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Abstract: By means of ab initio calculations with hybrid functionals we show a possibility for quasi-2D silicon structures originated from semiconducting Mg2Si, Ca2Si, Sr2Si and Ba2Si silicides to exist. Such a 2D structure is similar to the one of transition metal chalcogenides where silicon atoms form a layer in between of metal atoms aligned in surface layers. These metal surface atoms act as pseudo passivation species stabilizing crystal structure and providing semiconducting properties. Considered 2D Mg2Si, Ca2Si, Sr2Si and Ba2Si have band gaps of 1.14 eV, 0.69 eV, 0.33 eV and 0.19 eV, respectively, while the former one is also characterized by a direct transition with appreciable oscillator

strength. Electronic states of the surface atoms are found to suppress an influence of the quantum confinement on the band gaps. Additionally, we report Sr2Si bulk in the cubic structure to have a direct band gap of 0.85 eV as well as sizable oscillator strength of the first direct transition.

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