Quasi-2D silicon structures based on ultrathin Me_2Si (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 Mg_2Si, Ca_2Si, Sr_2Si and Ba_2Si 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 Mg_2Si, Ca_2Si, Sr_2Si and Ba_2Si have band gaps of 1.14eV, 0.69eV, 0.33eV and 0.19eV, 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 Sr_2Si bulk in the cubic structure to have a direct band gap of 0.85eV as well as sizable oscillator strength of the first direct transition.

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