Stability of 2D Alkaline-Earth Metal Silicides, Germanides and Stannides

A. Yu. Alekseev 1,

A. G. Chernykh 2,

A. B. Filonov 3,

D. B. Migas 4

N. V. Skorodumova (Foreign) 5

2019

1, 2, 3, 4 Department of Micro- and Nanoelectronics, Belarusian State University of Informatics and Radioelectronics, R&D Department, Center 4.11 "Nanoelectronics and new materials", R&D Lab 4.12 «Electrochemical nano-structure materials», Minsk, Belarus

5 Foreign (Multiscale Materials Modelling, Department of Materials and Engineering, Royal Institute of Technology (KTH), SE-10044 Stockholm, Sweden; Department of Physics and Astronomy, Uppsala University, Box 516, SE-75121 Uppsala, Sweden)

Keywords: 2D crystal, Silicide, Germanide, Stannide, Stability, Total energy, Phonon dispersion.

Abstract: By means of ab initio calculations, we have estimated stability of 2D Me_2X (Me = Mg, Ca, Sr, Ba and X = Si, Ge, Sn) in the T

and Td phases, which are similar to the ones of 2D transition metal chalcogenides, in addition to their phonon spectra. The T phase is found to be more stable for 2D Ca₂X, Sr₂X and Ba₂X, whereas the Td phase is predicted to be the ground state for 2D Mg₂X. We have also discussed that imaginary frequencies in the calculated phonon spectra of 2D Me₂X, which appeared in the vicinity of the _ point, were not necessarily associated with the dynamic instability.

This article published in: Stability of 2D Alkaline-Earth Metal Silicides, Germanides and Stannides / A. Yu. Alekseev [and others] // International Journal of Nanoscience – 2019. – Vol. 18, № 3-4. – P. 1940013. – https://doi.org/10.1142/S0219581X1940012X.

Internet link to the article:

https://www.worldscientific.com/doi/10.1142/S0219581X1940012X.

© 2019 World Scientific Publishing Co Pte Ltd. All rights reserved.