Lattice Design for Non-Carbon Two-Dimensional Allotropic Modifications

N.D. Abramenko and M.A. Rozhkov

ITMO University, Kronverksky pr., 49, St. Petersburg 197101, Russia

Abstract. In this article, an approach to lattice design for two two-dimensional allotropic materials is proposed. The approach is based on the use of crystal lattices of disclinated graphene known as pseudo-graphenes. The approach is demonstrated on pseudo-graphenes G5-7v1 and G5-6-7v2 and target crystals originated from molybdenum disulfide and phosphorene. Geometry optimization done by density functional theory calculations display that the designed lattices for new materials are structurally stable, which means that they could be synthesized and that the new approach could successfully be used to produce lattice designs for novel two-dimensional allotropic materials.

ACKNOWLEDGEMENTS
Fruitful discussions with Prof. A.E. Romanov and Prof. A.L. Kolesnikova are kindly acknowledged. The work was supported by Russian Science Foundation research project 19-19-00617.

REFERENCES


© 2021 ITMO