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Lattice Design for Non-Carbon Two-Dimensional Allotropic Modifications

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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 mo\lybdenum 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.

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