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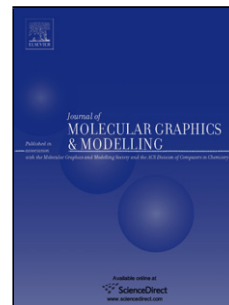
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Optimized Tersoff empirical potential for germanene

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Highlights

- The issue of re-parameterization of Tersoff empirical potential model was addressed for 2D nanomaterial ‘germanene’.
- Many properties of germanene were extracted using both original and optimized Tersoff potentials and they compared with the corresponding DFT data.
- The new optimized Tersoff potential introduced here provides a significant improvement in many structural, thermodynamic, mechanical, and thermal properties of germanene.

ABSTRACT

In the current work, the issue of re-parameterization of Tersoff empirical potential model was addressed for 2D nanomaterial ‘germanene’ to be applied in molecular dynamics simulation

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