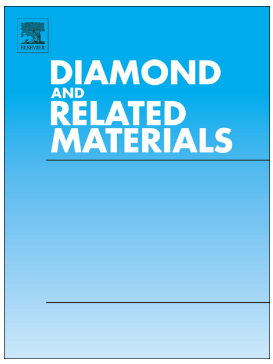

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Structural and electronic properties of two-dimensional (110) diamond nanofilms by first-principles calculations

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Abstract

Based on the first-principles calculations, we investigate the structural and electronic properties of pure and hydrogenated two-dimensional (2D) (110)-oriented diamond nanofilms related to the layer number (*n*). After structural optimization, for the pure (110) diamond nanofilms at n =1 and 2, the buckling 2D diamonds reconstruct into the planar graphene, and for the case of $n \geq 3$, the original diamond structures are energetically favorable to be maintained. The calculated electronic properties of these optimized structures show that the pure and semi-hydrogenated 2D diamond nanofilms have metallic characteristics, and the full-hydrogenated structures are semiconductors. It theoretically demonstrates that the *n* and surface functionalization could effectively modulate the structural and electronic properties of the 2D atomically thick (110) diamond nanofilms, revealing their applications in numerous practical fields especially fabricating low-dimensional optoelectronic devices.

Keywords: Two-dimensional (110) diamond nanofilms; First-principles calculations; Structural evolution; Electronic properties; Surface hydrogenation

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