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Vegard's Law in the Si_{1-y}C_y alloys

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Abstract : In this work, we presented a calculated of structural properties of the Si_{1-y}C_y binary alloys, the atomic structure of this alloys is important for understanding its properties. We used theories of bond-length of Vegard's approach based of the method of linear augmented plane wave (FP-LAPW) based on the theory of density functional (DFT). We also studied the structural properties of this alloys with the LDA approximation for the potential for exchange and correlation. Our study affirms that the lattice constant is approximately equal to the composition-weighted average of the lattice constants of the pure materials.

Keywords : Vegard's law, Structural properties, SiC