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Title: The investigation of the C-Si interface structure in Diamond/Si nano-composite films with first principle method

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Research Highlights

- > We investigate the stability of the monolayer Si interface on Diamond (001) surface.
- > The adsorption energies of the four kinds of 8C8Si configurations on diamond (001) surface were calculated by DFT.
- > The stability of the monolayer SiC interface on Diamond (001) surface is investigated.

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