

Abstract Submitted
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Stability of epitaxial graphene on pristine Si(111) BRANDEN KAPPES, TERESA DAVIES, Colorado School of Mines, SUKKY JUN, University of Wyoming, ADRI VAN DUIN, Penn State University, CRISTIAN CIOBANU, Colorado School of Mines — Incorporation of carbon nanostructures with silicon-based nanoelectronics will involve the direct integration of graphene with silicon chips, but so far graphene has not been grown on pristine silicon surfaces. Because usual synthesis routes would likely lead to the formation of silicon carbide, we calculate the binding energy of graphene transferred onto the Si(111) surface and also analyze its stability at various temperatures. Our calculations based on (commensurate) moiré superstructures with periodic boundary conditions show a strong graphene–substrate binding, about 1.5 eV/carbon atom, over a wide range of in-plane orientations of the graphene layer. Molecular dynamics simulations based on bond-order and reactive force field interatomic potentials suggest that the graphene binds to the substrate where carbon is rehybridized sp^3 , and that this rehybridized graphene structure does not lead to the decomposition of graphene into silicon carbide even at temperatures as high as 80% of the substrate melting temperature.

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