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Insights into the epitaxial growth of graphene on SiC substrate: A computational study MING YU, C.S. JAYANTHI, S.Y. WU, University of Louisville — Experimentally, the epitaxial growth of graphene on SiC substrate has been observed for both the Si-terminated (0001) or C-terminated $(000\bar{1})$surface of 4H-SiC or 6H-SiC wafers, respectively at sufficiently high temperatures in ultra-high vacuum [Surface Science **600**, 3906 (2006); PRB **77**, 155303 (2008)]. However, the mechanism of the sublimation of Si atoms and the graphitization of excess C atoms on the surface of 4H-SiC or 6H-SiC wafers that leads to the epitaxial growth of graphene on SiC is still unclear. The purpose of this work is to conduct a temperature-dependent study of the evolution of 4H-SiC surfaces using the molecular dynamics scheme based on the SCED-LCAO Hamiltonian [PRB **74**, 155408 (2006)] so that the evolution of the surface reconstruction of 4H-SiC including the formation of the interface between the substrate and graphene layers can be understood at the microscopic level.

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