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Interfacial Structures of Graphene on 4H- SiC Substrates: SCED-LCAO Molecular Dynamics[1] MING YU, University of Louisville, SEAN FANCHER, Purdue University, JOSEPH H. BUTERA, C.S. JAYANTHI, S.Y. WU, University of Louisville — The purpose of this work is to obtain a microscopic understanding of the interface between the graphene and Si-terminated as well as C-terminated 4H-SiC substrates by studying several cases of nearly commensurate overplayed structures. Relative energies of these different structures are calculated using the SCED-LCAO method [PRB **74**, 15540; PHYSE **42**,1] to gain insight into the role played by the lattice mismatch in releasing the strain and thus lowering the energy of the system. Further insight into the interfacial properties is obtained by analyzing the local strain in terms local atomic and bonding arrangements [PRB **59**, 7745] which will be correlated to the lattice mismatch. Our results will be compared with current experimental [PRL **100**, 176802; PRB **77**, 155303; J. Phys: Condens Matter **21**, 134016; PRB **78**, 205424; J. Phys: Condens Matter **20**, 323202] and theoretical [PRL **99**, 076802; PRL **99**, 126805; PRB **77**, 235412; PRL **100**, 176802] results.

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