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Electronic Properties of Epitaxial Graphene on Si(111)-7×7 and 3CS-SiC(100) Substrates SHU XU, North Carolina State University, THUSHARI JAYASEKERA, Southern Illinois University, MARCO BUONGIORNO NARDELLI, North Carolina State University — The synthesis of epitaxial graphene is an attractive method for industrial-scale fabrication and mass production of graphene-based electronic devices. Recently, efforts of epitaxial growth of graphitic carbon films on Si(111)-7×7 and 3CS-SiC(100) substrates have been undertaken in order to explore new potential substrates compatible with conventional Si technology. In this talk, we will discuss the electronic properties of epitaxial graphene on Si (111)-7×7 and 3CS-SiC(100) substrates using calculations from first principles based on Density Functional Theory. In particular, we found that a single graphene layer on Si(111)-7×7 displays ripples of about 0.5 Å and shows an n type electronic behavior. We also calculated the band structures for a graphene bilayer on 3CS-SiC(100) surface with different staking sequences. While AA stacking on Si face and turbostratic stacking on C face show n type behavior, turbostratic stacking on Si face and AA stacking on C face show p type behavior. On both faces, the first carbon plane is covalently bonded to the substrate and serves as a buffer layer similarly to the graphene/6H-SiC(0001) system previously studied.

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