

Abstract Submitted
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**Structural Properties of Epitaxial Graphenes on 4H-SiC(0001):
A Theoretical Study**¹ MING YU, PAUL DAVIS, MICHAEL WOODCOX, C.S.
JAYANTHI, S.Y. WU, University of Louisville — The structural properties of the
epitaxial graphene including the buffer layer on 4H-SiC(0001) are studied using
the recently developed SCED-LCAO molecular dynamics scheme [PRB 74, 15540
(2006)]. Both Si-terminated and C-terminated SiC substrates are considered. In a
previous work [BAPS, Vol. 56, 463 (2011)], we had shown that 10x10 monolayers
of carbon on 8x8 4H-SiC(0001) substrate as well as 13x13 monolayers of carbon on
 $6\sqrt{3}\times 6\sqrt{3}$ 4H-SiC(0001) substrate are minimum in strain between the buffer layer
and the substrate and that they are nearly commensurate. In this work, we have
added an epitaxial layer of graphene to the above geometries and both C-terminated
and Si-terminated SiC surfaces will be considered. We will highlight the roles played
by the buffer layer, the epitaxial layer, and the substrate on the structural properties
of this system. Analysis of the structure in terms of local bonding arrangements and
charge distributions will also be provided.

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