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Carbon-Rich Silicon Carbide XIAO SHEN, YEVGENIY PUZYREV, Vanderbilt University, GERD DUSCHER, University of Tennessee-Knoxville, SOKRATES PANTELIDES, Vanderbilt University — The application of SiC in electronic devices is currently hindered by low carrier mobility at the the SiO_2/SiC interfaces. Recently, it was found that thermally grown SiO_2/4H-SiC interface can have a transition layer on the SiC side with C/Si ratio as high as 1.2[1] and the channel mobility of the fabricated SiC MOSFETs decreases as the thickness of the transition layer increases.[2] However, the atomic structure of the transition layer is unknown. Here we present the results of first-principles calculations for silicon carbide with 20% excess carbon. Both static density functional theory calculations and quantum molecular dynamics simulations were performed. We reveal the structure that forms when a large amount of excess carbon is incorporated into the lattice. In addition we explore pairing and cluster formation. The overall results will be assessed against experimental data. This work is supported in part by NSF GOALI grant DMR-0907385.

[1]T. Zheleva, et. al. APL 93, 022108 (2008)
[2]T. L. Biggerstaff, et. al. APL 95, 032108 (2009)

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