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Atomistic modeling of amorphous silicon carbide: A first-principles study[1] PARTHAPRATIM BISWAS, University of Southern Mississippi, RAYMOND ATTA-FYNN, University of Texas, Arlington — Localized basis *ab initio* molecular dynamics techniques within density functional theoretic framework have been used to model a realistic atomistic configuration of amorphous silicon carbide (a-$Si_{0.5}C_{0.5}$) containing 1000 atoms. The structural, electronic and vibrational properties have been studied and compared to existing theoretical models and available experimental data. Our study clearly reveals that the short-range chemical order in this material is predominant due to presence of heteronuclear Si-C bonds with coordination defect concentration less than 5% and the chemical disorder parameter was $\chi = 0.083$. Our 1000-atom model shows the presence of a clean gap in the spectrum and we also study the nature of the localization of the electronic band tail states as well as the vibrational eigenmodes.

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