Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Structural and electronic properties of amorphous silicon carbide: A first principles and experimentally constrained molecular relaxation approach[1] PARTHAPRATIM BISWAS, The University of Southern Mississippi, RAYMOND ATTA-FYNN, University of Texas at Arlington — We present first-principles modeling of amorphous silicon carbide within a localized basis density functional formalism to study the electronic, vibrational and structural properties for system containing 1000 atoms. Our work for $Si_{.5}$-$C_{.5}$ system shows that the short range chemical order is dominated by heteronuclear Si-C bonds with coordination defect with a degree of chemical disorder. We calculate the electronic density of states that shows a presence of clean optical gap in the spectrum and study the localization nature of the electronic band tail states and vibrational eigenstates. We compare our results with existing models and experimental data available in the literature. Finally, we presents some preliminary results for models obtained by experimentally constrained molecular relaxation technique [1,2] that directly uses experimental data in conjunction with a classical force-field.
[1] P. Biswas, D.N. Tafen and D.A. Drabold, Phys Rev B71, 54204
[2] P. Biswas, R. Atta-Fynn, S. Chakraborty, and D.A.Drabold, J.Phys.:Condens. Matter 19 (2007) 455202

[1]University of Southern Mississippi, Grant No. DE00945.

Parthapratim Biswas
The University of Southern Mississippi

Date submitted: 03 Dec 2007 Electronic form version 1.4