Abstract Submitted
for the TSS18 Meeting of
The American Physical Society

Stability prediction and electronic properties study of silicon-rich silicon carbide NOURA ALKHALDI, MUHAMMAD N. HUDA, Department of Physics, The University of Texas at Arlington — Silicon-rich silicon carbide structures which are thermodynamically stable can be used in applications without requiring a pure grade of Silicon or pure grade of silicon carbide materials. Density functional theory (DFT) calculations were used to examine the stability of various structures of silicon carbide in order to produce stable structures of silicon-rich silicon carbide materials. Since we found that changing the configuration of carbon atoms which are replaced by silicon atoms play a significant role in getting stable structures as well as lower band gaps, we investigated different configurations of silicon and carbon atoms in these silicon carbide structures to obtain suitable silicon-rich silicon carbide materials with tailored band gaps. We have studied the electronic structures of these structures as well.

Noura Alkhaldi
Department of Physics, The University of Texas at Arlington

Date submitted: 12 Mar 2018 Electronic form version 1.4