

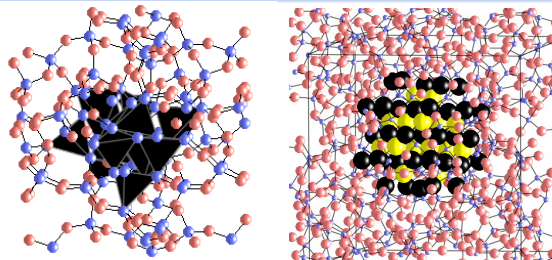
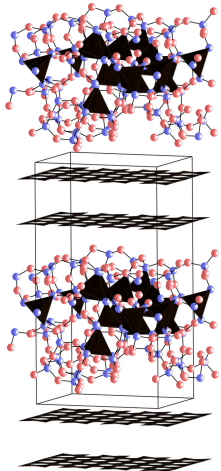
Collaborative Research: NanoDomain Structure and Multifunctional Properties of Polymer Derived Ceramics

Peter Kroll, DMR 0907117 [Rishi Raj, DMR 0907108]

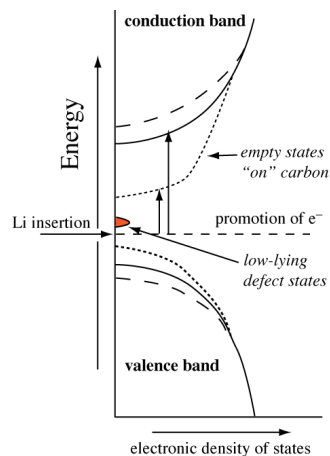
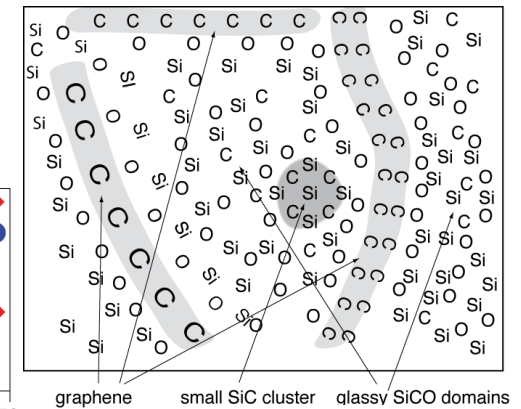
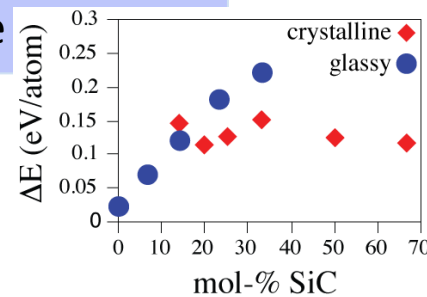
Goal: atomistic simulations to clarify microscopic structure of amorphous SiCO ceramics
Method: density functional calculations and extensive network modeling

Structure & Energy

- SiC clusters precipitate in silica glass
- “C-rich” interface SiCO-C & “bonded” C-SiO₂ interface energetically not favorable
- no “stable” ternary SiCO structure



revised “Nanodomain model”



SiCO as novel Li-Anode material

- Li bonds cationic Li⁺-O => e⁻ to unoccupied states
 - “irreversible” Li attached to C-defects
 - fortuitous balance between Li⁺-O and electron promotion allows Li doping up to 1 Li per C !
- ⇒ defect-free C-rich SiCO for best anode material

