INTRODUCTION

SiC is a very popular semiconductor material which has over 200 polymorphs available such as 3C, 2H, 4H, 6H, 8H,10H according to their stacking pattern of Si and C bilayers.¹ It is well known for its reliability in extreme environments and high-performance applications, due to properties like,

- High Band Gap
- High electric field strength
- High breakdown voltage
- High thermal conductivity, which makes it suitable for hightemperature and high-power applications.²

Previous studies have demonstrated that doped SiC is a promising candidate for photovoltaic applications.³

MOTIVATION

- SiC has a bandgap of 2.3–3.3 eV, which is higher than the ideal range for efficient solar absorption (<1.5 eV).⁴
- Non-stoichiometric silicon carbide (SiC) materials, especially silicon-rich SiC, are tailored to reduce SiC's high bandgap and to enhance solar light absorption efficiency.⁵
- First-principles calculations have demonstrated that silicon-rich silicon carbide (SiC) nanoclusters exhibit structural stability and possess tunable energy gaps.⁶
- To explore the potential of non-stoichiometric SiC in the bulk phase, we investigated silicon-rich SiC by substituting carbon atoms with silicon within different configurations of silicon carbide (SiC) using density functional theory.

METHODOLOGY

- principles calculations are performed with density • First functional theory (DFT). DFT is based on Hohenberg-Kohn theorem which states that if we know the ground state electron density of a system, we can determine its ground state thermodynamic properties uniquely.
- The interaction between core and valence electrons are treated by the projector augmented wave (PAW) method along with Perdew-Burke-Ernzerhof (PBE) functional for exchange-correlation interaction.
- The kinetic energy cutoff for the plane waves is set to 550 eV.
- Convergence criterion for the self-consistent calculations is 10⁻⁷ eV for the total energy.
- Brillouin zone integration is performed using the tetrahedron method.
- The calculations are performed with the Vienna ab initio simulation package (VASP).
- All computations are performed at the Texas Advanced Computing Center (TACC).



Silicon-rich SiC for efficient Solar Energy Absorption

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Formation Enthalpy:

The formation enthalpy was calculated using the following formula, $\Delta H_{f} = E(Si_{x}C_{y}) - xE(Si) - yE(C)$



Formation enthalpy of Silicon-rich SiC:

- Chemical formula of silicon-rich SiC is nSi_c:SiC which states n number of **carbon** atoms are replaced by **n** number of silicon atoms in a pristine SiC.
- We replaced up to 3 carbon atoms by silicon.
- Si substitution leads to an increase in the lattice parameters compared to the pristine structure due to the prevalence of Si–Si bonds, which have a longer bond length than Si–C bonds.
- Our investigation found that, substituted silicon atoms (considering the position of image as well) tend to stay closely, which results in the lowest formation enthalpy and thus the most stable arrangement.
- For example, in pristine 8H-SiC supercell, three substituted Si atoms in carbon sites yields a lower formation enthalpy (-0.073 eV) when they were substituted closer than when they were placed apart (-0.071 eV).

• Si substitution introduces defect states in the band structure, and when Si atoms are in close proximity, these states strongly interact.

• The interaction between closely spaced Si atoms enhances the overlap of impurity states, leading to a more significant band gap reduction compared to when they are farther apart.

(a) Band Structure for pristine 8H-SiC (3x3x1 supercell)

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(c) PDOS plot for 8H 2Si_c.SiC (near center)



**Contribution from the doped atom was amplified by 10 times

RESULT and DISCUSSION

Band Gap:

Our calculated band gap for different SiC polymorphs aligns with existing experimental and theoretical studies, while also reflecting the known limitation of GGA in underestimating band gaps.

Changes in Band Gap due to extra silicon substitution



Band Gap of silicon-rich SiC:



RESULTS and DISCUSSION

(b) PDOS plot for 8H 1Si_c.SiC



(d) PDOS plot for 8H 3Si_c.SiC (near center)



RESULT and DISCUSSION

(b) Band Structure for 8H 1Si_c.SiC



(c) Band Structure for 8H $3Si_{C}$.SiC (forming a line near center)



CONCLUDING REMARKS

• Substituted silicon atoms prefer to stay closely which leads to the lowest formation enthalpy and the most stable configuration.

• Partial Density of States (PDOS) analysis shows that the dominant contribution near the Fermi level originates from the p orbitals of the doped Si atoms.

• The band gap can be tailored by substituting Si atom on C sites in the pristine SiC structures.

• To achieve a band gap value that closely aligns with existing experimental results, hybrid functional calculations are currently being performed.

• Overall, tailoring the band gap by replacing Si on C sites in SiC makes it more useful in the realm of SiC based optoelectronic devices and solar cell applications.