Hydrogen Enhances Radiation Resistance of Amorphous Silicon Oxycarbide

– Hepeng Ding, et al.

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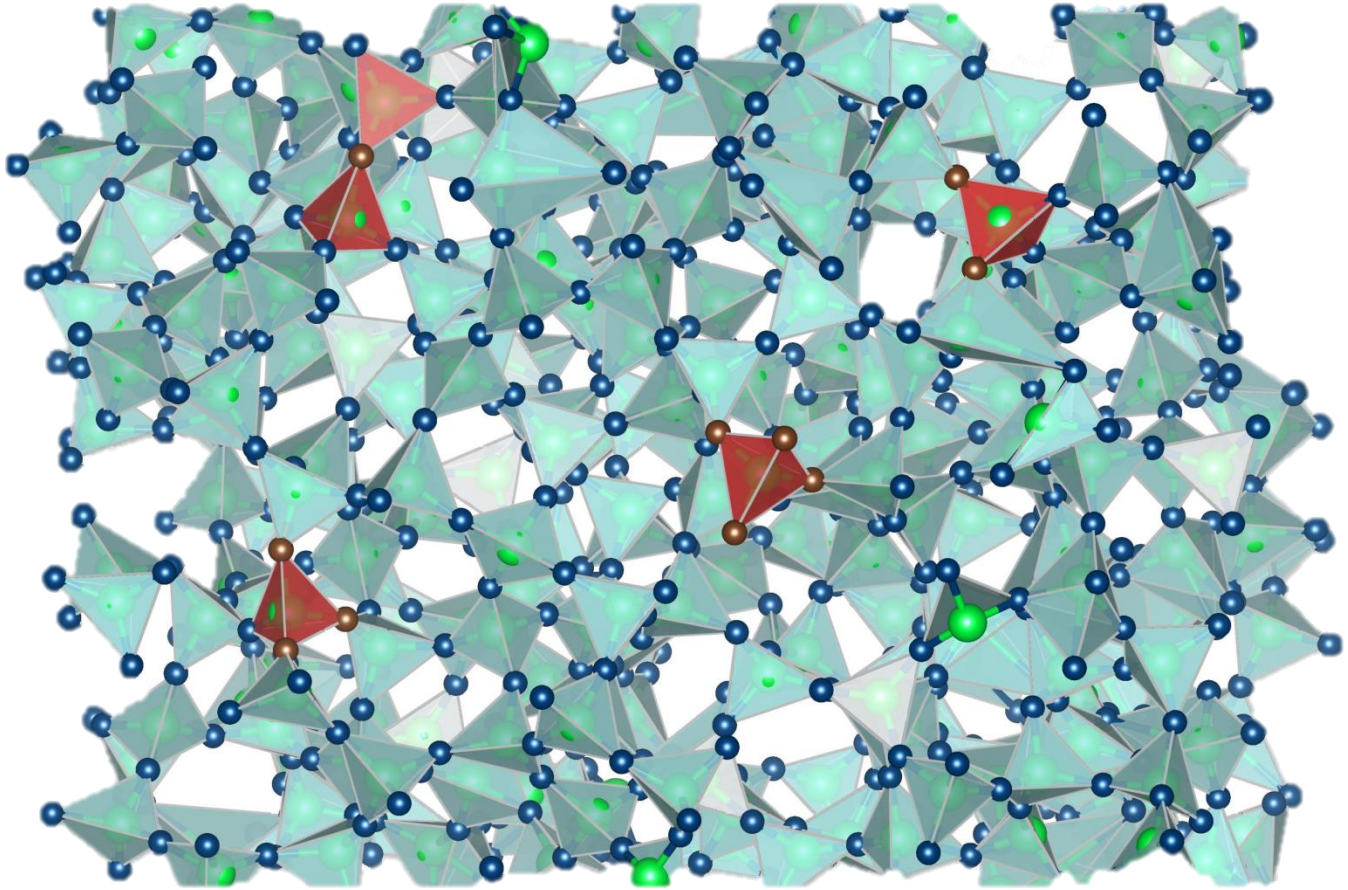
Introduction

Silicon oxycarbide (SiOC): a class of thermally stable amorphous solids

Amorphous: no translational symmetry, therefore no traditional point defects upon ion irradiation



Continuous Random Network (CRN) of SiOC

What is the radiation response of SiOC?

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Computational Methods

- Classical potential MD: LAMMPS/ReaxFF
- First principles DFT: VASP/PAW-PBE/550 eV
- Unit displacement damage ---
  100 eV primary knock-on atom (PKA)

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Highlights

- Conducted the first ever first principles MD studies of radiation knock-on damage in amorphous solids
- H reverses the C clustering tendency in SiOC
- H enhances the radiation resistance of SiOC ---

  Fully hydrogenated SiOC is “radiation indifferent”

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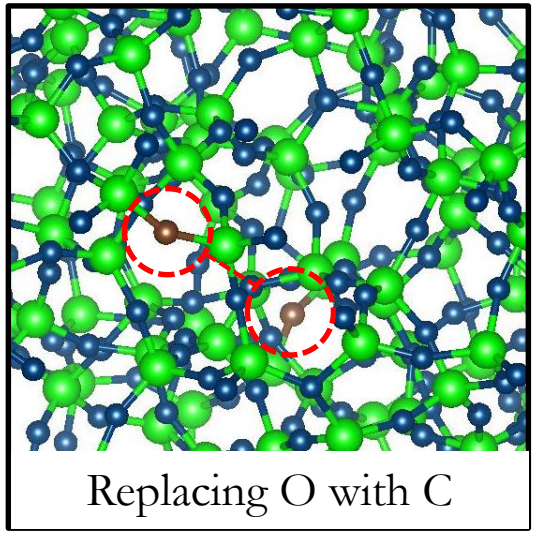
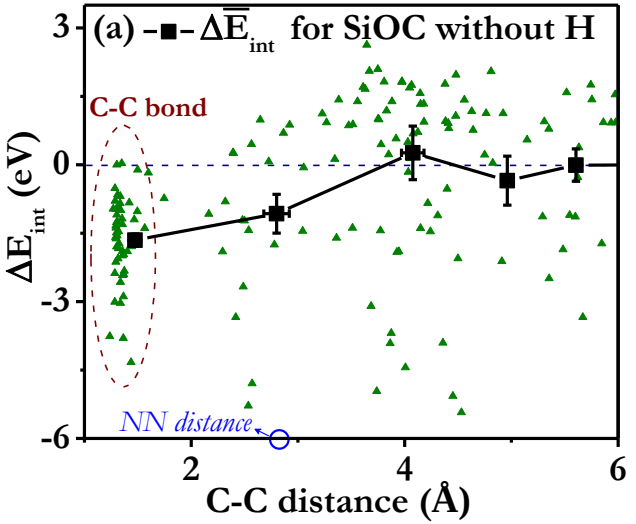
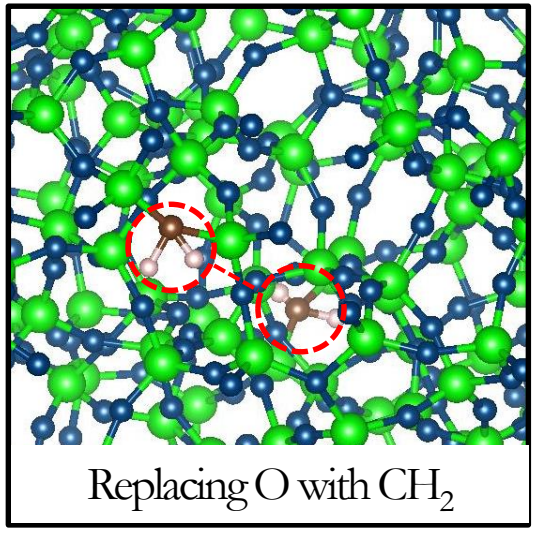
Result and Discussion

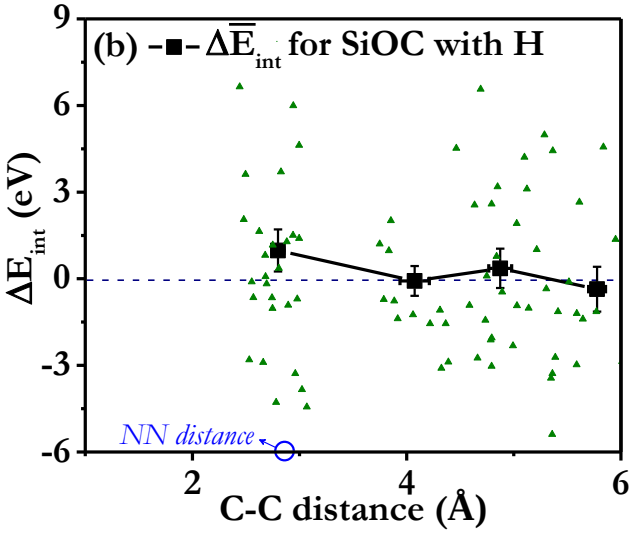
- Constructing an atomic model of SiOC

H reverses C-C interaction: attractive to repulsive


Replacing O with C




Replacing O with CH_2



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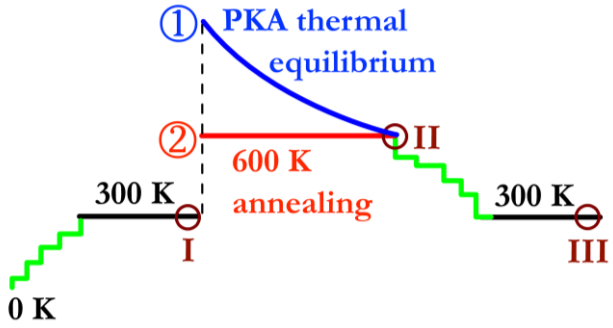
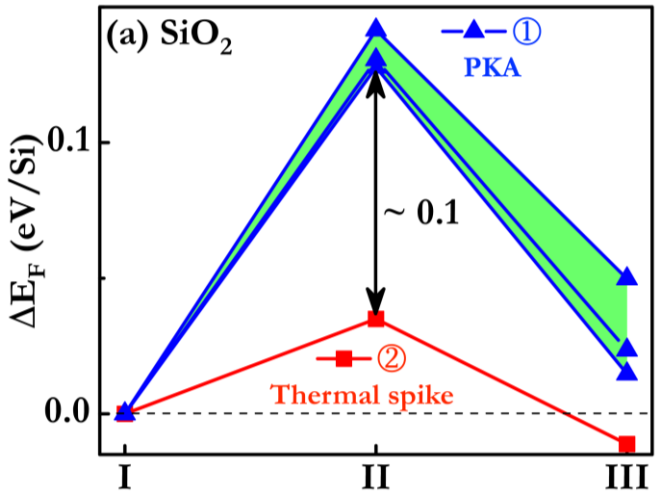
Result and Discussion

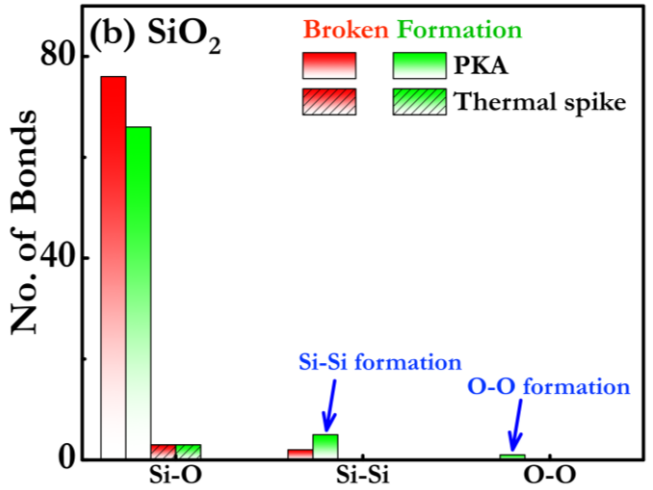
❖ Investigating radiation response of SiOC

PKA (Process 1)
=
Thermal spike (Process 2)
+
Atom displacement



➢ SiO2: decreased stability; bond defect formation





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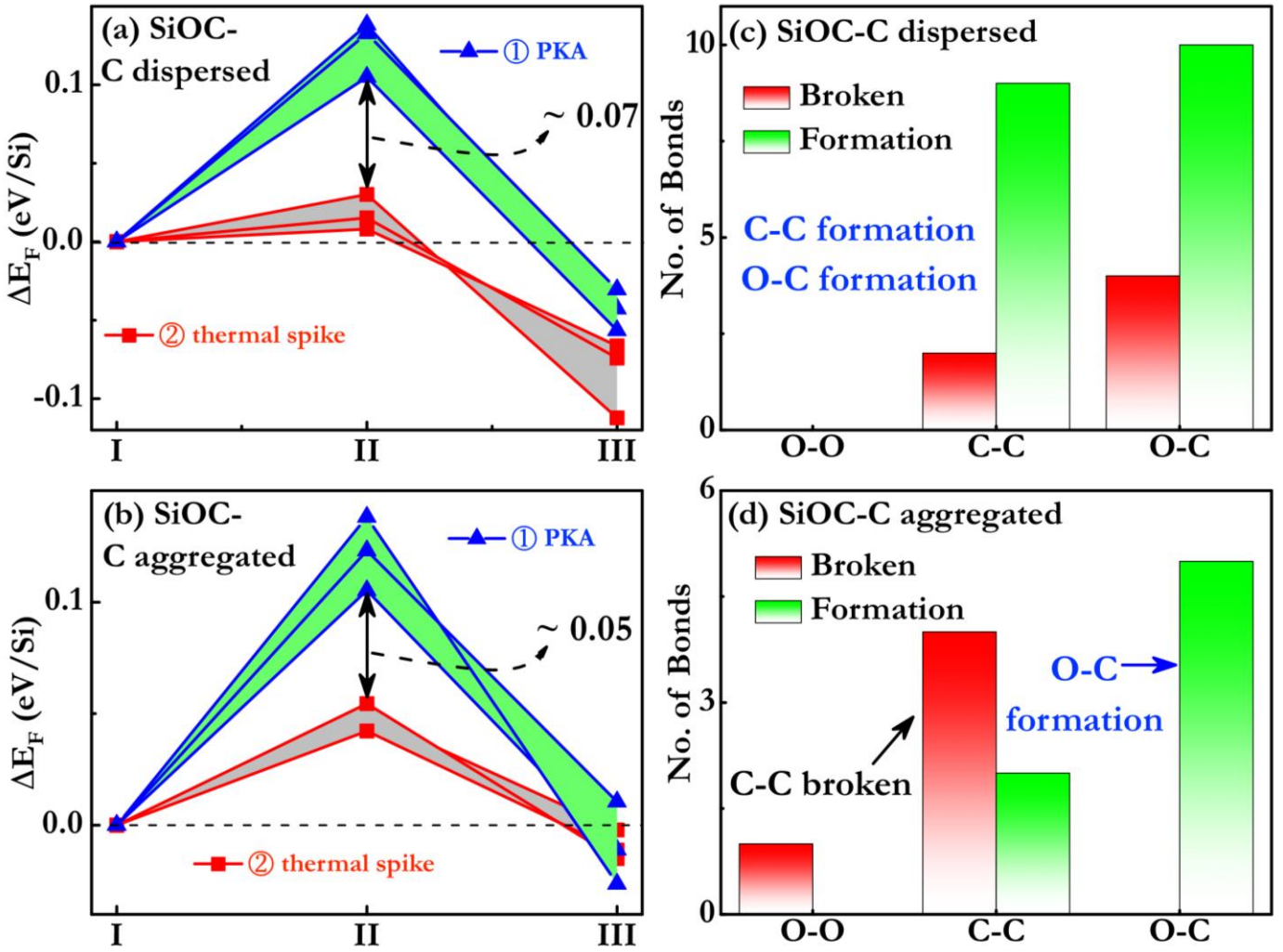
Result and Discussion

- SiOC --- effect of C
  - Conserved thermal stability
  - Decreased atom displacement effect
  - Changed C distribution: C-C bond change
  - Decreased C concentration: O-C bond formation



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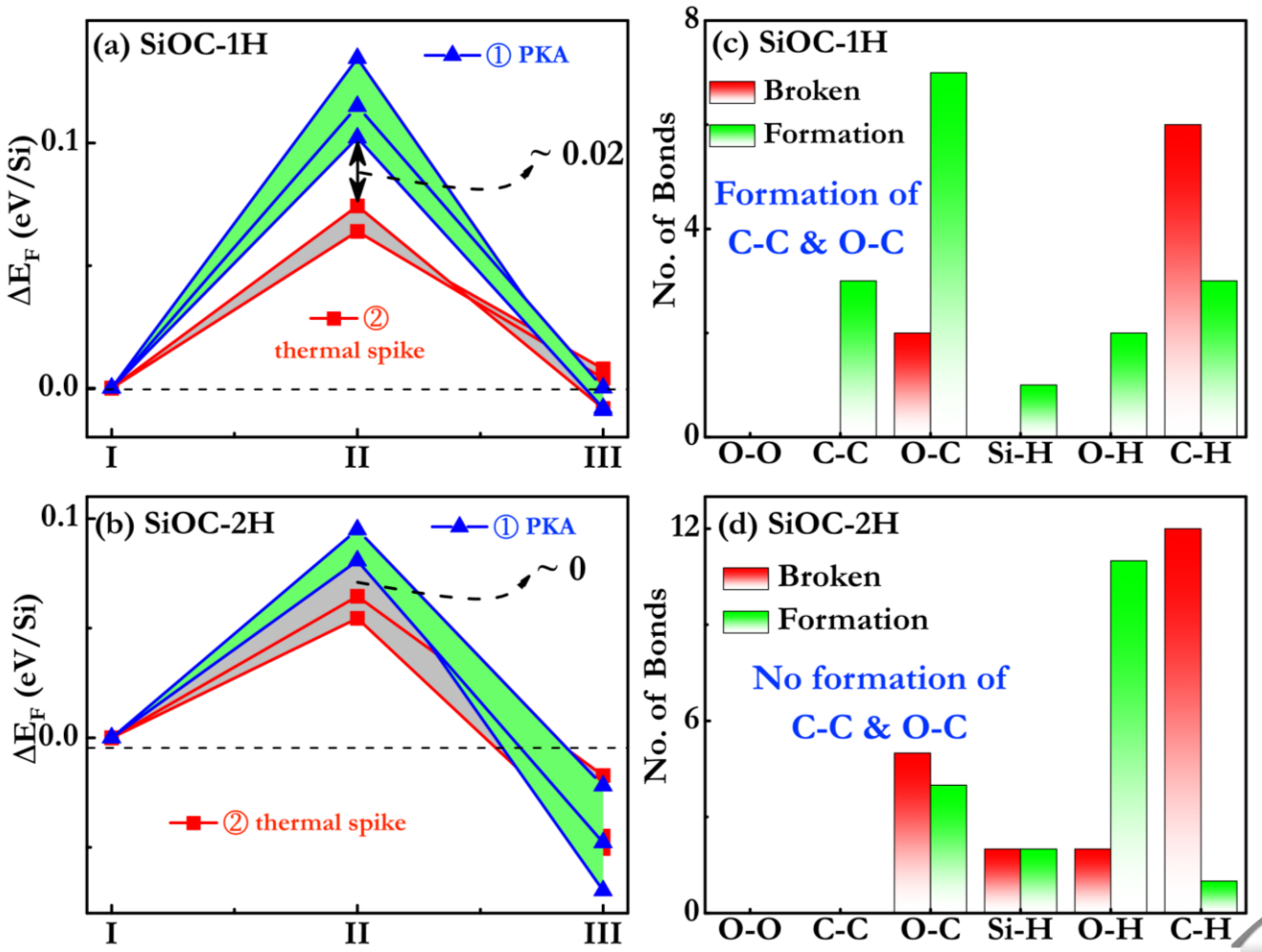
Result and Discussion

➢ Hydrogenated SiOC --- effect of H

Negligible atom displacement effect in SiOC-2H

Conserved C distribution and concentration in

SiOC-2H: no change on C-C and O-C bonds



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Note and Acknowledgement

- First principles DFT is used for the properties of the materials that we interested. A typical job contains ~1000 atoms, with ~300 cores and ~1 GB memory/core and run time of one week.
- We thank the computational resources provided by the Texas A&M High Performance Research Computing program.
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