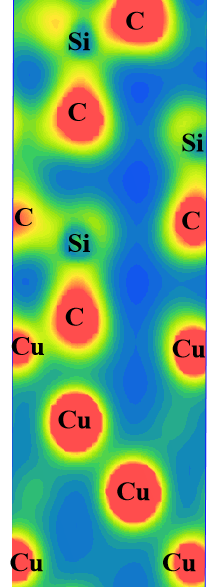
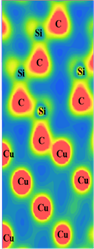
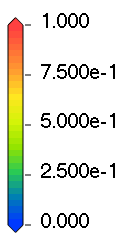
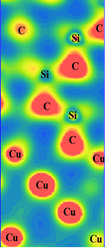
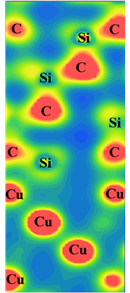
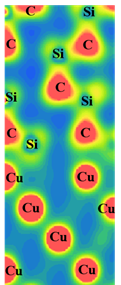
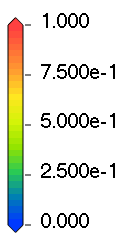
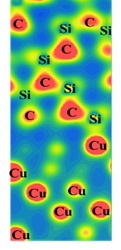
**Supplementary Information**

Interfacial Stabilities, Electronic Properties and Interfacial Fracture Mechanism of 6H-SiC Reinforced Copper Matrix studied by the First Principles Method

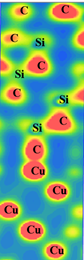
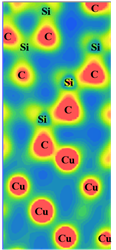
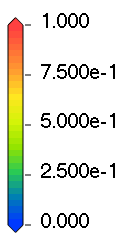
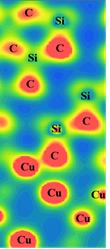
  

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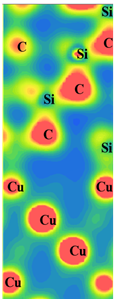
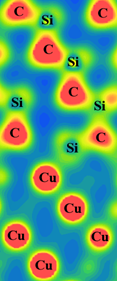
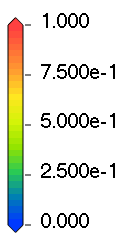
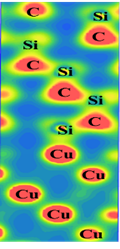
  

**(d)** CT-HCP(b) **(e)** CT-MT(b) **(f)** CT-OT(b)

**FIG. SI(1).** The charge density distribution of the interfacial atoms of all “(b)” type of 6H-SiC(0001)/Cu(111) interfacial models along (211) interfaces (eV/Å3)

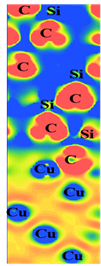
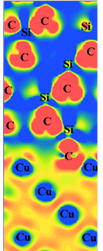
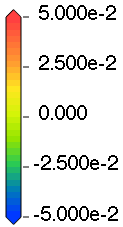
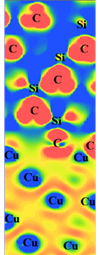
  

**(a)** CT-HCP(c) **(b)** CT-MT(c) **(c)** CT-OT(c)

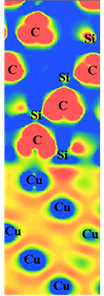
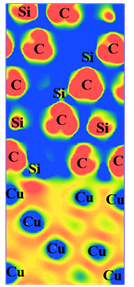
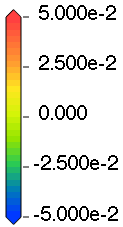
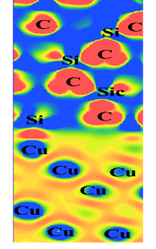
  

**(d)** CT-HCP(c) **(e)** CT-MT(c) **(f)** CT-OT(c)

**FIG. SI(2).** The charge density distribution of the interfacial atoms of all “(c)” type of 6H-SiC(0001)/Cu(111) interfacial models along (211) interfaces (eV/Å3)

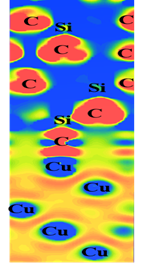
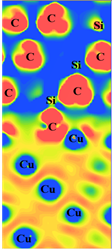
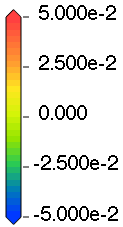
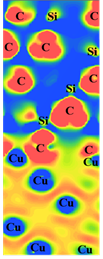
  

**(a)** CT-HCP(b) **(b)** CT-MT(b) **(c)** CT-OT(b)

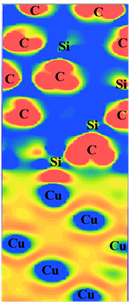
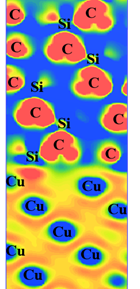
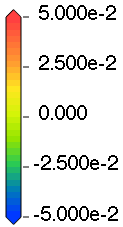
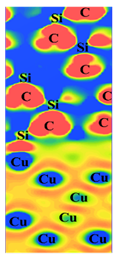
  

**(d)** CT-HCP(b)  **(e)** CT-MT(b)  **(f)** CT-OT(b)

**FIG. SI(3).** The charge density difference of the interfacial atoms of all “(b)” type of 6H-SiC(0001)/Cu(111) interfacial models along (211) interface (eV/Å3).

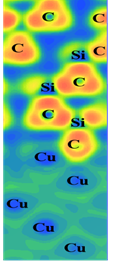
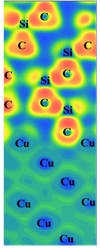
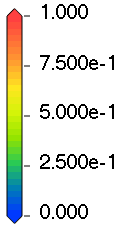
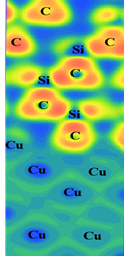
  

**(a)** CT-HCP(c)  **(b)** CT-MT(c) **(c)** CT-OT(c)

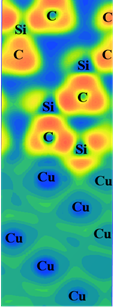
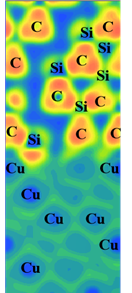
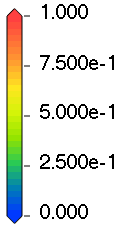
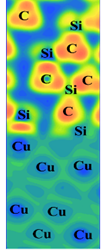
  

**(d)** CT-HCP(c) **(e)** CT-MT(c) **(f)** CT-OT(c)

**FIG. SI(4).** The charge density difference of the interfacial atoms of all “(c)” type of 6H-SiC(0001)/Cu(111) interfacial models along (211) interface (eV/Å3).

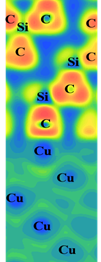
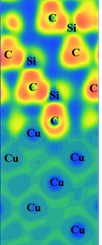
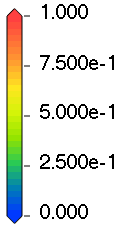
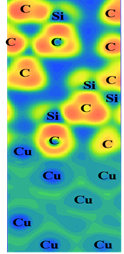
  

**(a)** CT-HCP(b) **(b)** CT-MT(b) **(c)** CT-OT(b)

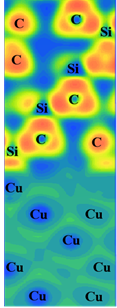
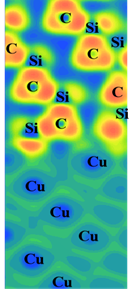
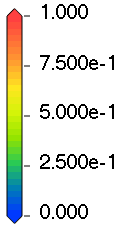
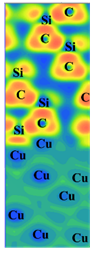
  

**(d)** CT-HCP(b) **(e)** CT-MT(b) **(f)** CT-OT(b)

**FIG. SI(5).** The electron localization function of the interfacial atoms of all “(b)” type of 6H-SiC(0001)/Cu(111) interfacial models along (211) interface (eV/Å3).

**(a)** CT-HCP(c) **(b)** CT-MT(c) **(c)** CT-OT(c)

**(d)** CT-HCP(c) **(e)** CT-MT(c)  **(f)** CT-OT(c)

**FIG. SI(6).** The electron localization function of the interfacial atoms of all “(c)” type of 6H-SiC(0001)/Cu(111) interfacial models along (211) interface (eV/Å3).

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**(a)**CT-HCP(b) **(b)**CT-MT(b)

I:\data SiC-Cu processing\PDOS\CT\CT-OT\CT-OT-1\CT-OT-1-new-.tifI:\data SiC-Cu processing\PDOS\ST\ST-HCP\ST-HCP-1\ST-HCp-1-new.tif

**(c)**CT-OT(b) **(d)**ST-HCP(b)

I:\data SiC-Cu processing\PDOS\ST\ST-MT\ST-MT-1\ST-MT-1-new-.tifI:\data SiC-Cu processing\PDOS\ST\ST-OT\ST-OT-1\ST-OT-1-new-.tif

**(e)**ST-MT(b) **(f)**ST-OT(b)

**FIG. SI(7).** The partial density of state of the interfacial atoms of all “(b)” type of 6H-SiC(0001)/Cu(111) interfacial models.

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**(a)**CT-HCP(C) **(b)**CT-MT(c)

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**(c)** CT-OT(c) **(d)**ST-HCP(c)

I:\data SiC-Cu processing\PDOS\ST\ST-MT\ST-MT-2\ST-MT-2-news-.tifI:\data SiC-Cu processing\PDOS\ST\ST-OT\ST-OT-2\ST-OT-2-new-.tif

**(e)**ST-MT(c) **(f)**ST-OT(c)

**FIG. SI(8).** The partial density of state of the interfacial atoms of all “(c)” type of 6H-SiC(0001)/Cu(111) interfacial models.