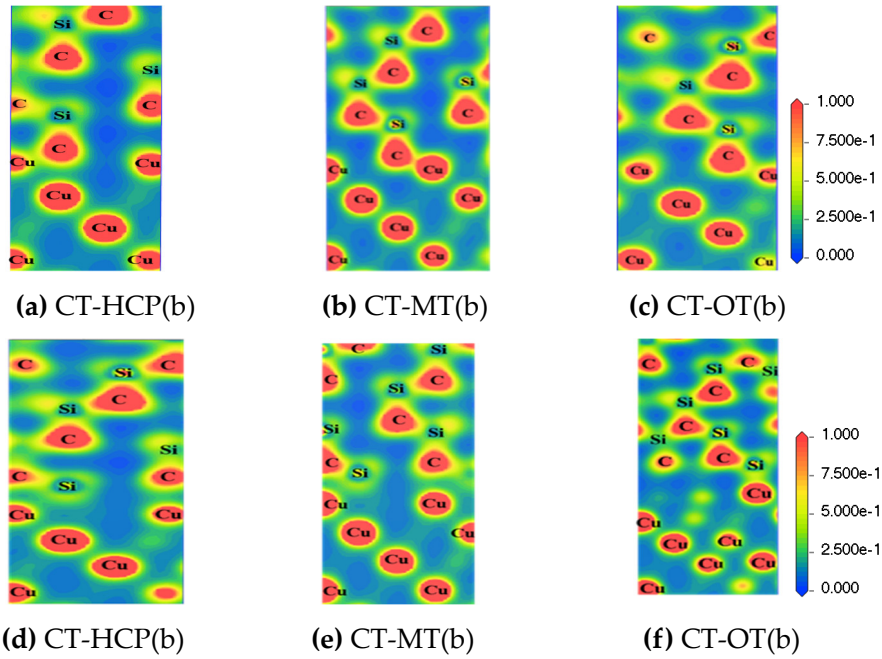
Supplementary Materials

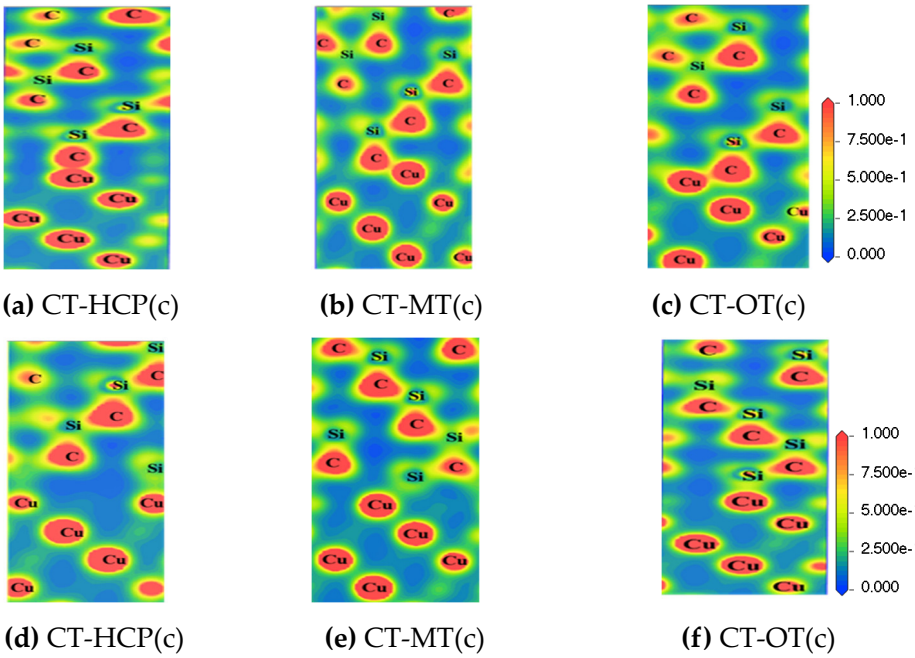
Interfacial Stabilities, Electronic Properties and Interfacial Fracture Mechanism of 6H-SiC Reinforced Copper Matrix studied by the First Principles Method



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

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

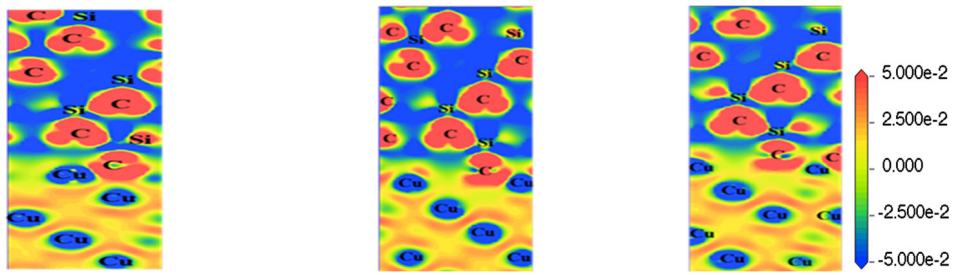
Figure S1. The charge density distribution of the interfacial atoms of all "(b)" type of 6H-SiC(0001)/Cu(111) interfacial models along (211) interfaces (eV/Å^3)



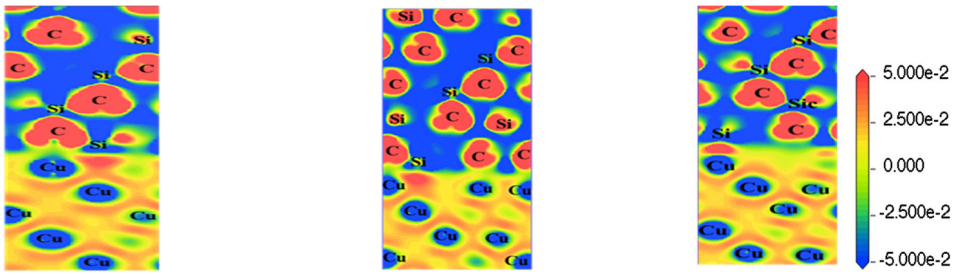
(a) CT-HCP(c) **(b)** CT-MT(c) **(c)** CT-OT(c)

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

Figure S2. The charge density distribution of the interfacial atoms of all "(c)" type of 6H-SiC(0001)/Cu(111) interfacial models along (211) interfaces (eV/Å^3)

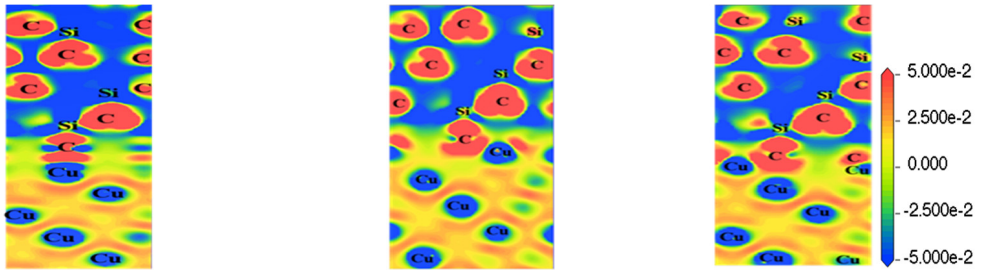


(a) CT-HCP(b) **(b)** CT-MT(b) **(c)** CT-OT(b)

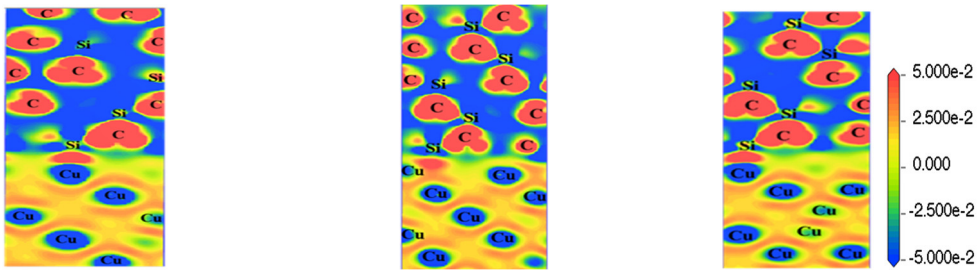


(d) CT-HCP(b) **(e)** CT-MT(b) **(f)** CT-OT(b)

Figure S3. The charge density difference of the interfacial atoms of all "(b)" type of 6H-SiC(0001)/Cu(111) interfacial models along (211) interface (eV/Å^3).

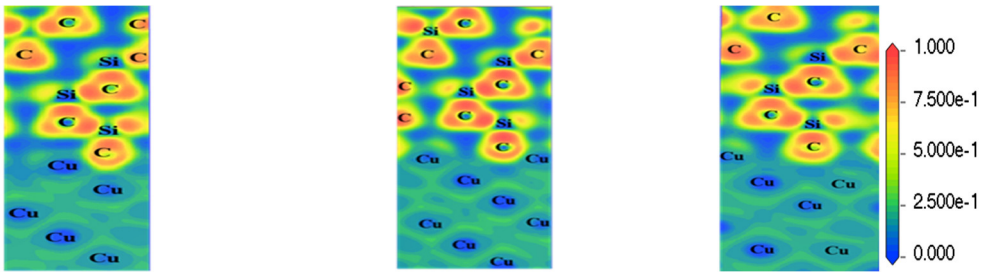


(a) CT-HCP(c) **(b)** CT-MT(c) **(c)** CT-OT(c)

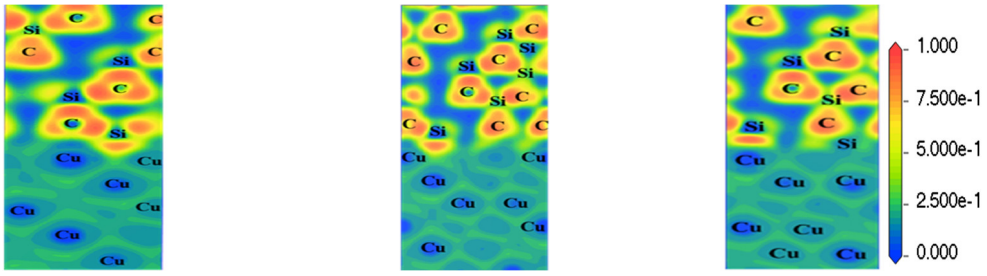


(d) CT-HCP(c) **(e)** CT-MT(c) **(f)** CT-OT(c)

Figure S4. The charge density difference of the interfacial atoms of all "(c)" type of 6H-SiC(0001)/Cu(111) interfacial models along (211) interface (eV/Å^3).

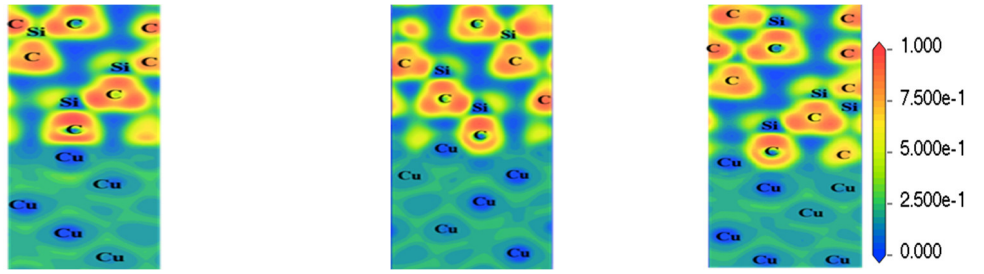


(a) CT-HCP(b) **(b)** CT-MT(b) **(c)** CT-OT(b)

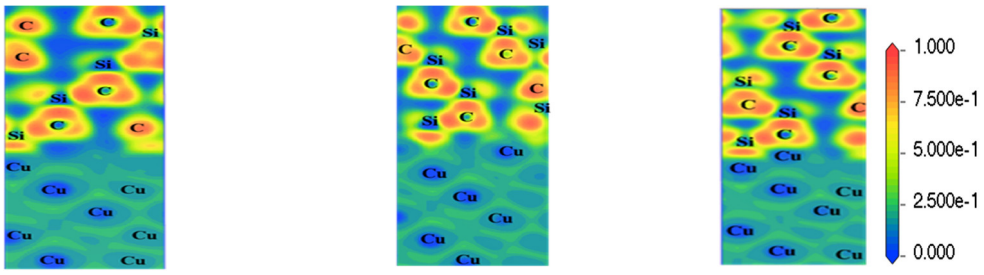


(d) CT-HCP(b) **(e)** CT-MT(b) **(f)** CT-OT(b)

Figure S5. The electron localization function of the interfacial atoms of all "(b)" type of 6H-SiC(0001)/Cu(111) interfacial models along (211) interface (eV/Å^3).

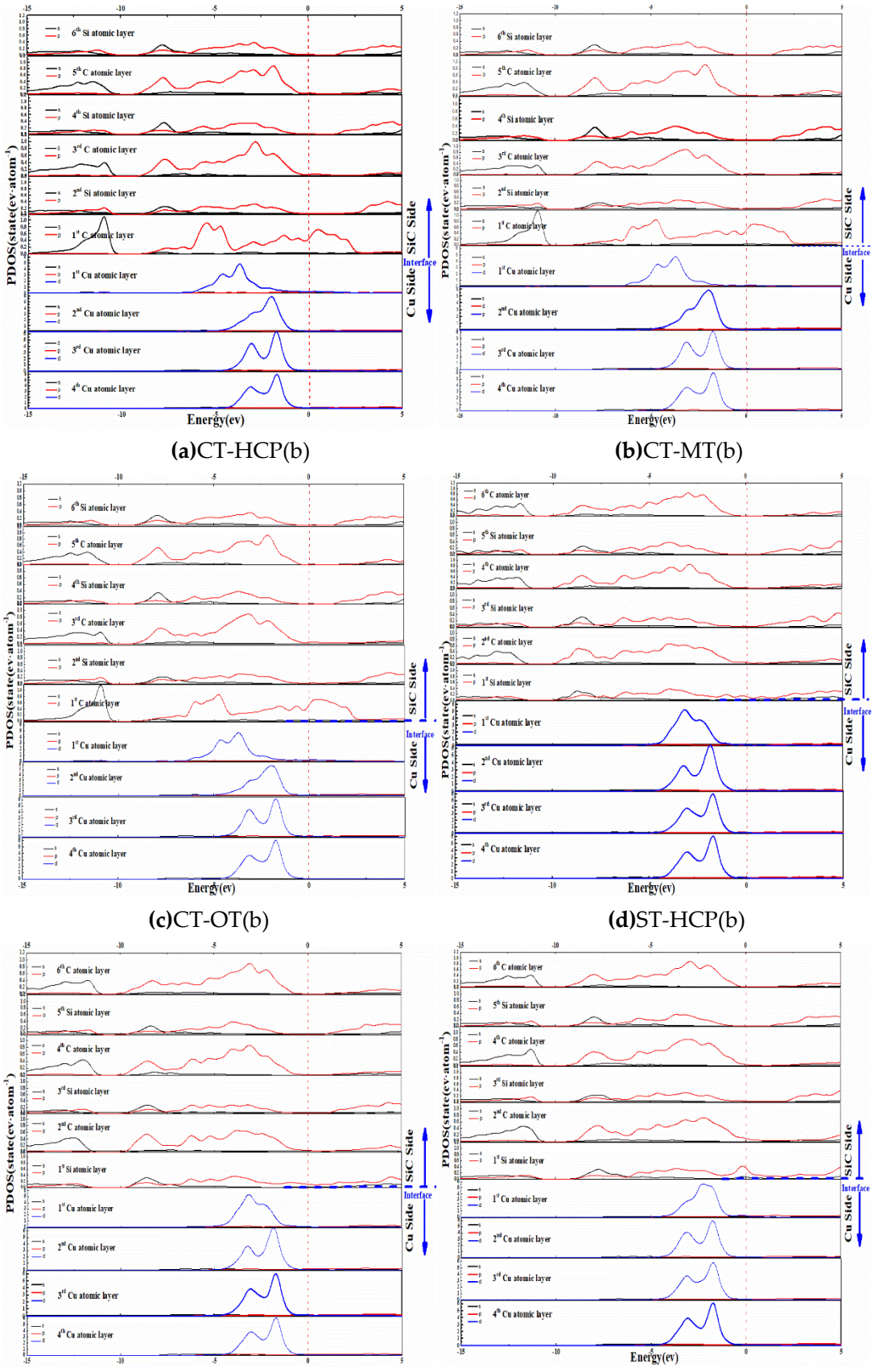


(a) CT-HCP(c) **(b)** CT-MT(c) **(c)** CT-OT(c)



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

Figure S6. The electron localization function of the interfacial atoms of all "(c)" type of 6H-SiC(0001)/Cu(111) interfacial models along (211) interface (eV/Å^3).

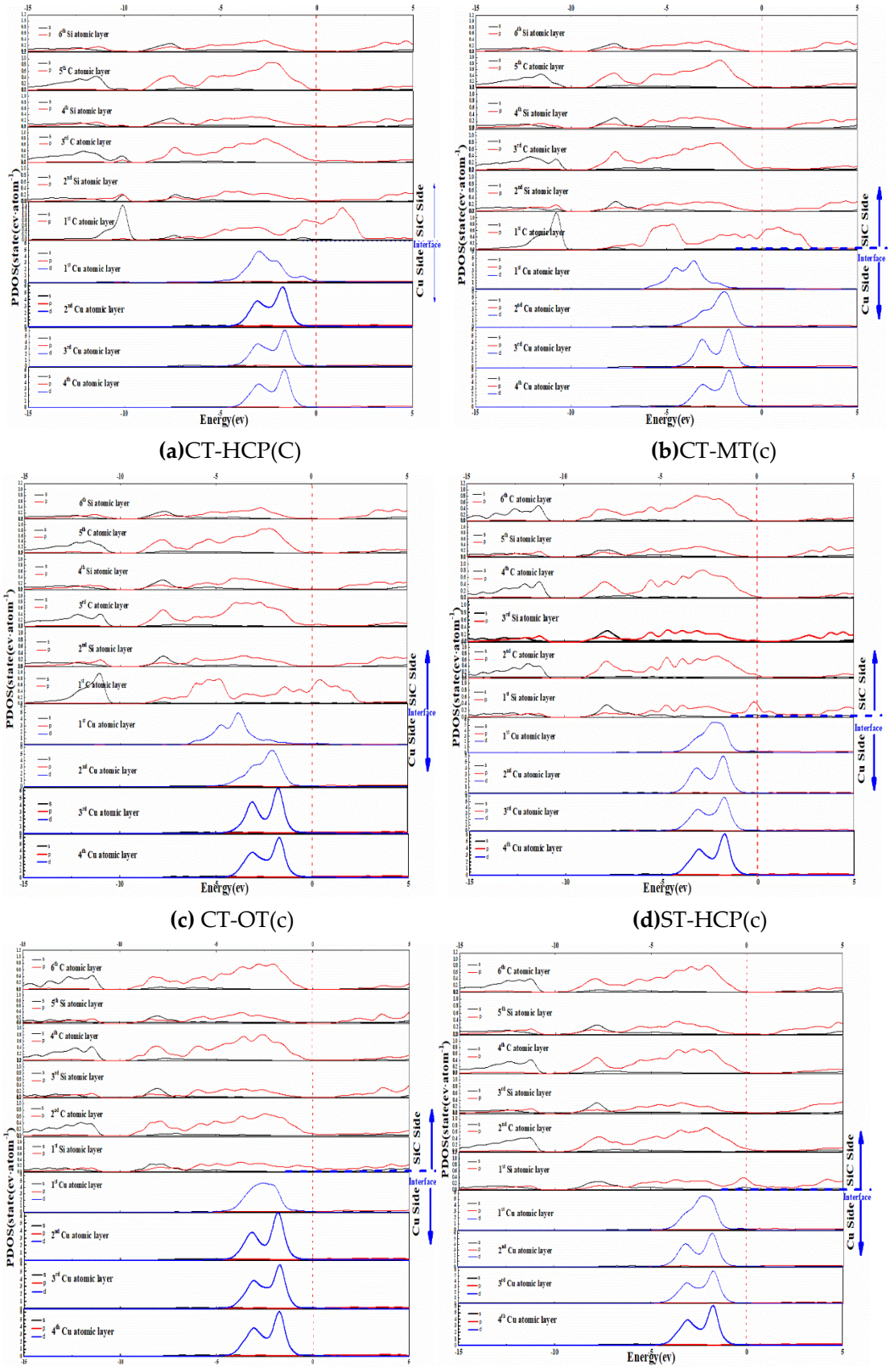


(a)CT-HCP(b) **(b)**CT-MT(b)

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

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

Figure S7. The partial density of state of the interfacial atoms of all "(b)" type of 6H-SiC(0001)/Cu(111) interfacial models.



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

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

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

Figure S8. The partial density of state of the interfacial atoms of all "(c)" type of 6H-SiC(0001)/Cu(111) interfacial models.