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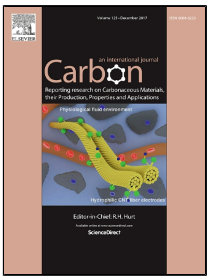

Adhesive transfer at copper/diamond interface and adhesion reduction mechanism with fluorine passivation: A first-principles study

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Graphical Abstract

1.The interfacial structure change, electronic and mechanical properties of Cu/diamond and interface with fully F passivation (Cu/diamond:F) have been evaluated through first-principles calculations.

2.The study shows that Cu(111)/diamond(111) interface exhibits the special phenomenon of adhesive transfer due to adhesion, and this contribute to different frictional properties among soft metal.

3.Passivation of fluorine on diamond surface reduces work of separation of the Cu/diamond interface significantly, from 3.64J/m^2 to 0.02J/m^2.

4.We also gain that fluorine might be a kind of promising adhesion-reducing element at interface and improve related tribological characteristics of Cu(111)/diamond(111) system.

5.The results of this study benefit the understanding of different tribological properties of Cu/DLC system, adhesion reduction mechanism of fluorine at interface and its effect on tribological behavior at atomic scale.