Supplementary Information for "Density functional theory study of high-energy metal (Al, Mg, Ti, and Zr)/CuO composites"

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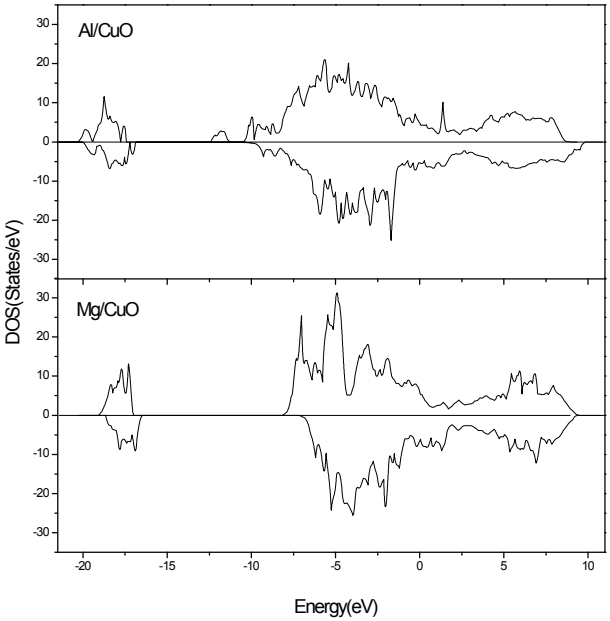
Table S1 Relaxed lattice constants of bulk CuO together with experimental and other calculated data.

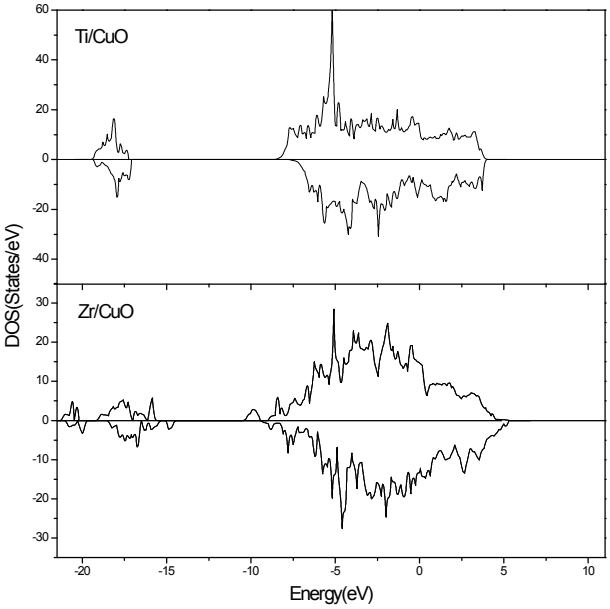
	a (Å)	b (Å)	c (Å)	β (°)
Expt.[31]	4.684	3.423	5.129	99.54
Expt.[32]	4.685	3.428	5.123	99.54
GGA+U[18]	4.76(1.6%)	3.48(1.7%)	5.21(1.6%)	99.50(-0.1%)
LSDA+U[33]	4.55(-2.9%)	3.34(-2.4%)	4.99(-2.7%)	99.51(-0.1%)
This work (PBE+U)	4.678(-0.1%)	3.366(-1.7%)	5.112(-0.3%)	99.80(0.3%)

Table S2 Adsorption energies of different number of close-packed Al layers with the closest layer located in the O_{suf} atom as shown in Figure 1(b).

Number of Al layers (4 Al per layer)	E_{ads} (eV)
One	-2.99
Two	-1.60
Three	-1.42
Four	-1.33
Five	-1.21
Six	-1.10

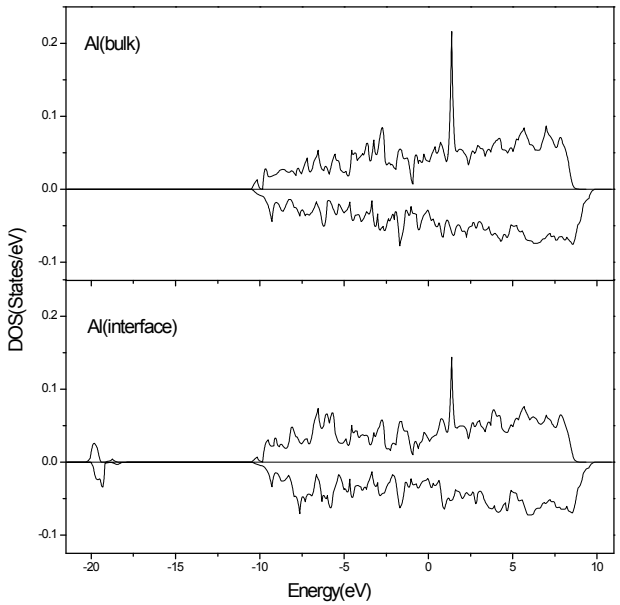

Al/CuO
Mg/CuO
DOS(States/eV)
Energy(eV)

28

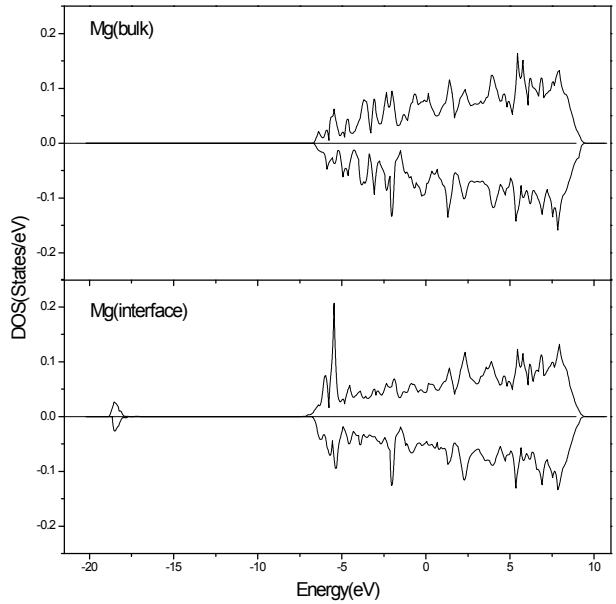

Ti/CuO
Zr/CuO
DOS(States/eV)
Energy(eV)

29

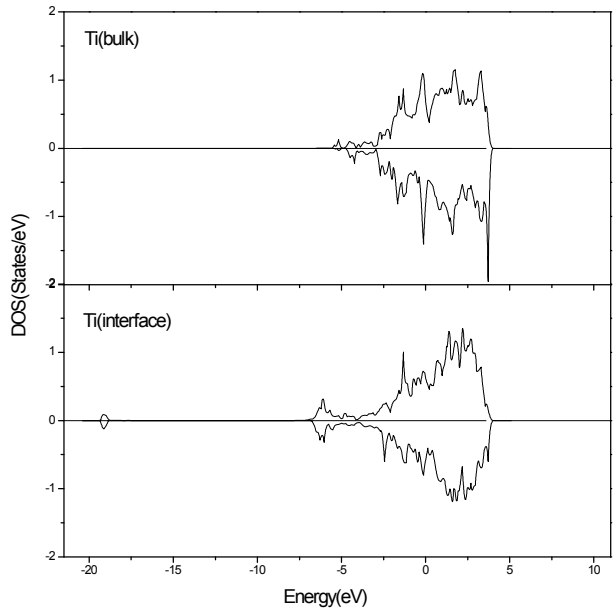
30 (a)


Al(bulk)
Al(interface)
DOS(States/eV)
Energy(eV)

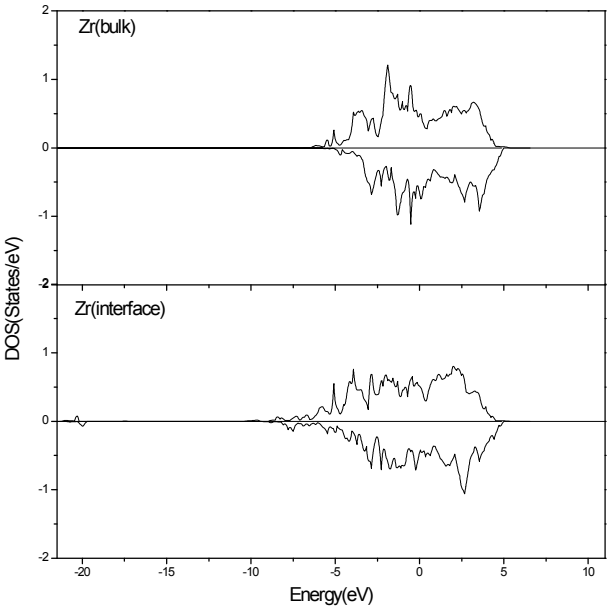
31


Mg(bulk)
Mg(interface)
DOS(States/eV)
Energy(eV)

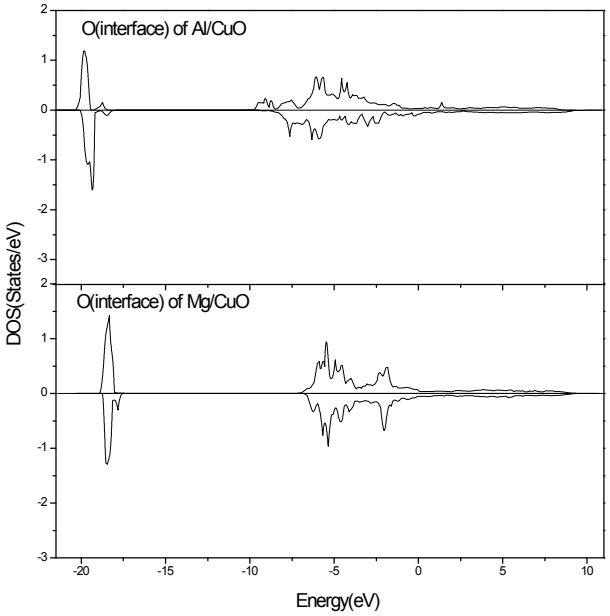
32

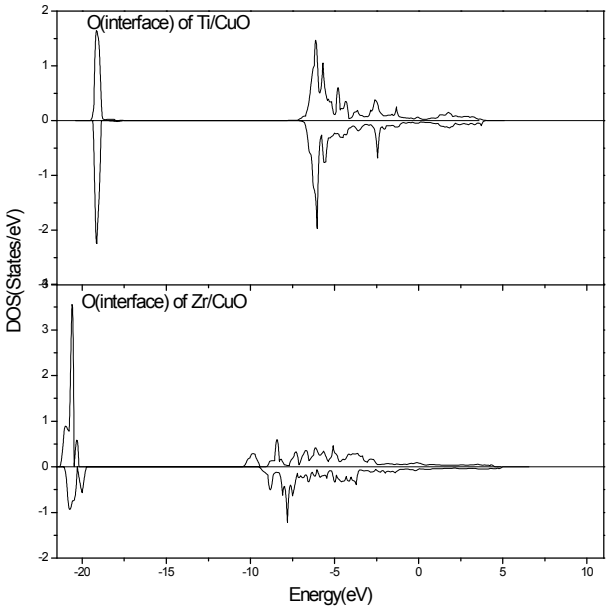

Ti(bulk)
Ti(interface)
DOS(States/eV)
Energy(eV)

33


Zr(bulk)
Zr(interface)
DOS(States/eV)
Energy(eV)

(b)


O(interface) of Al/CuO
O(interface) of Mg/CuO
DOS(States/eV)
Energy(eV)



(c)

Fig. S1 Calculated TDOS (a) and atom-projected PDOS (b) and (c) profiles for Al/CuO(111), Mg/CuO(111), Ti/CuO(111), and Zr/CuO(111). DOS for the atoms around the centers of metal layers (denoted as "bulk") and for interfacial metal and O in the on-top configuration are displayed. The Fermi level of each supercell is set at 0 eV.