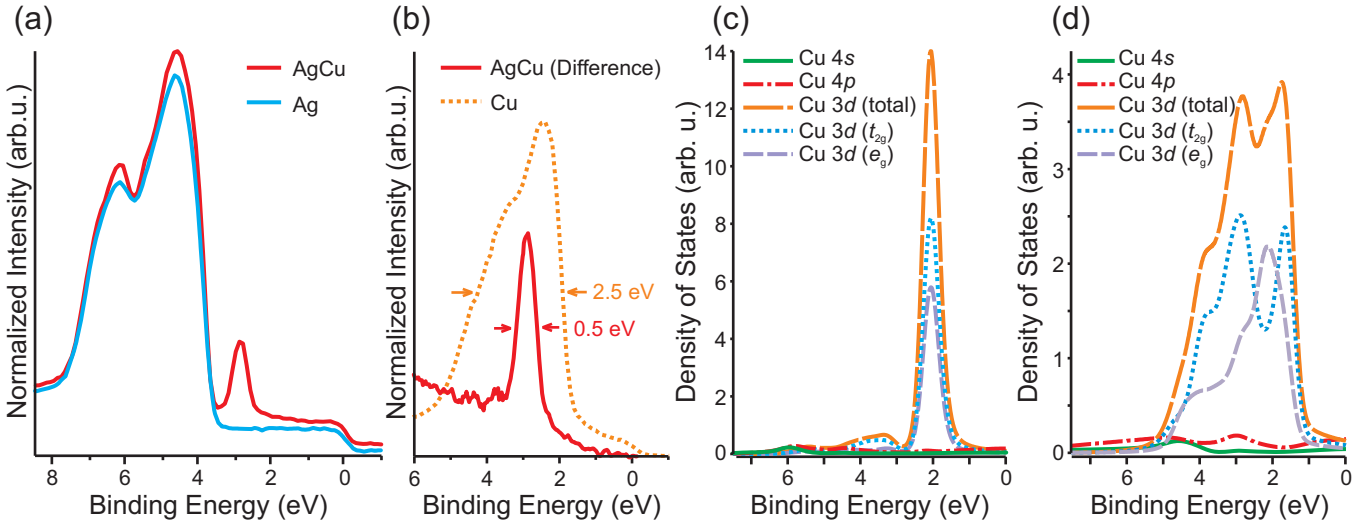
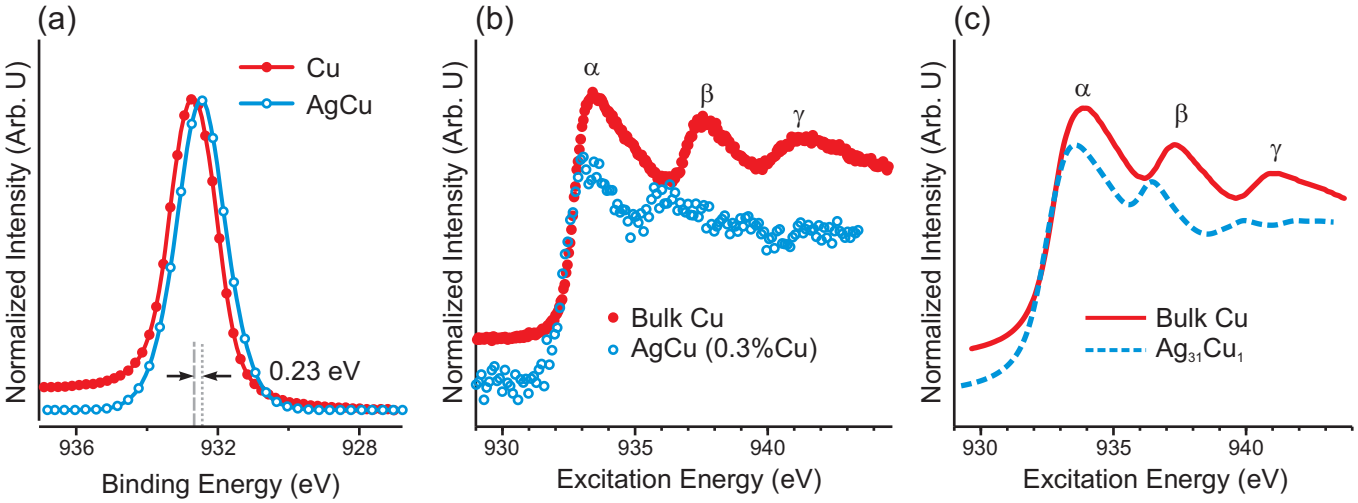
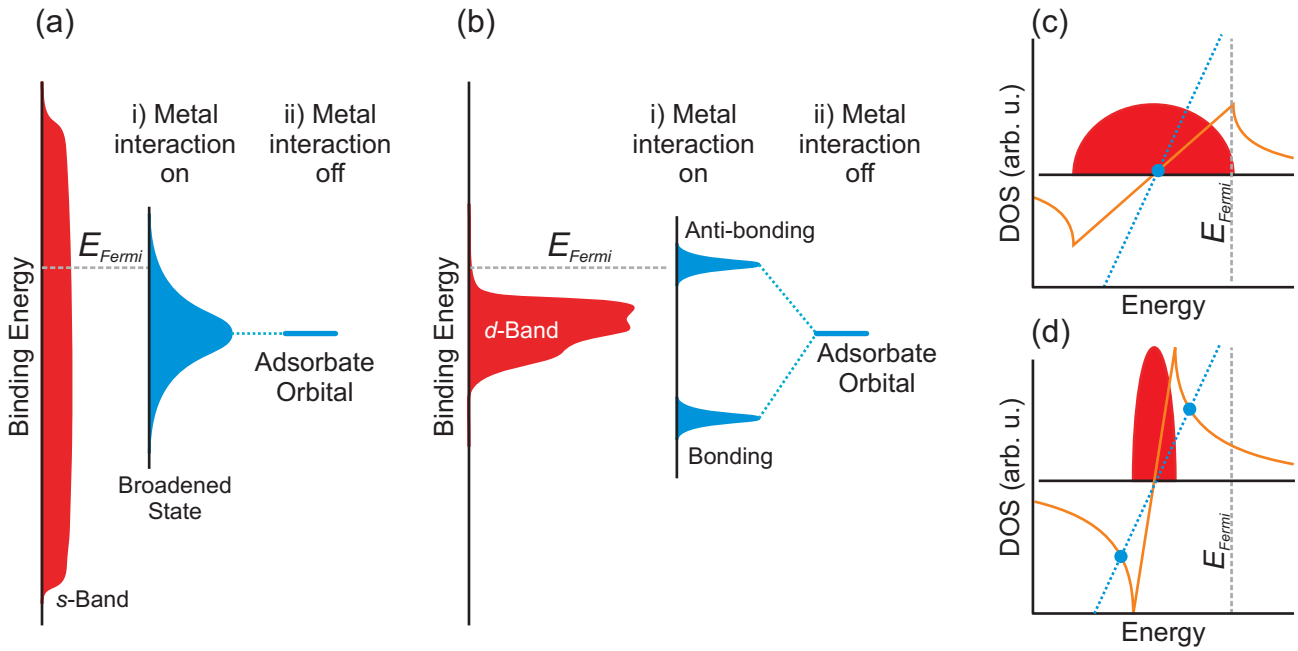
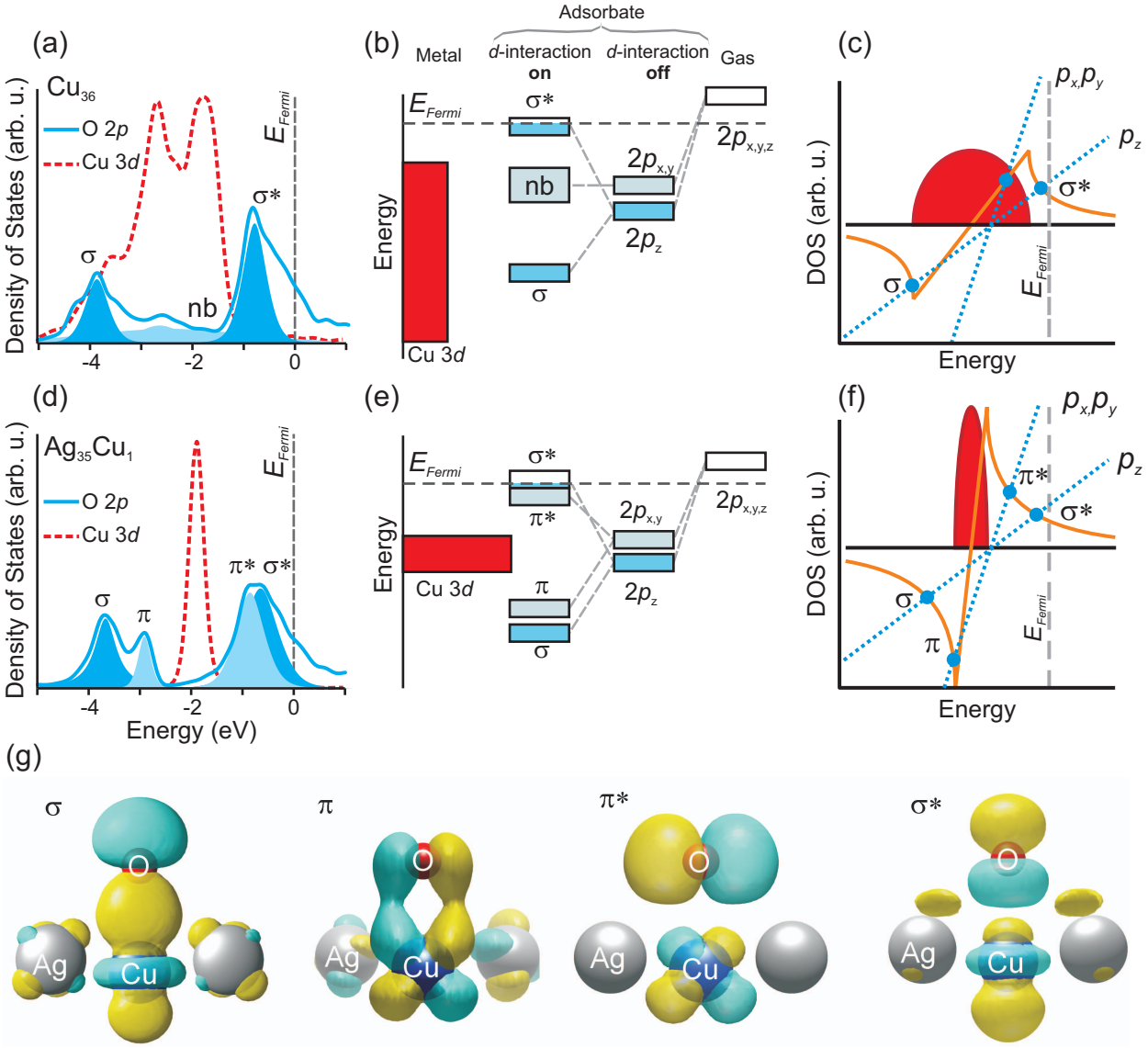
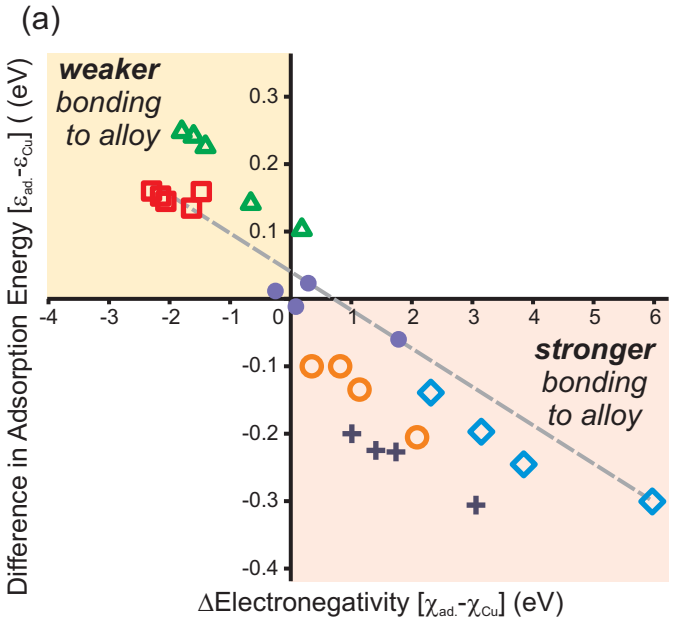
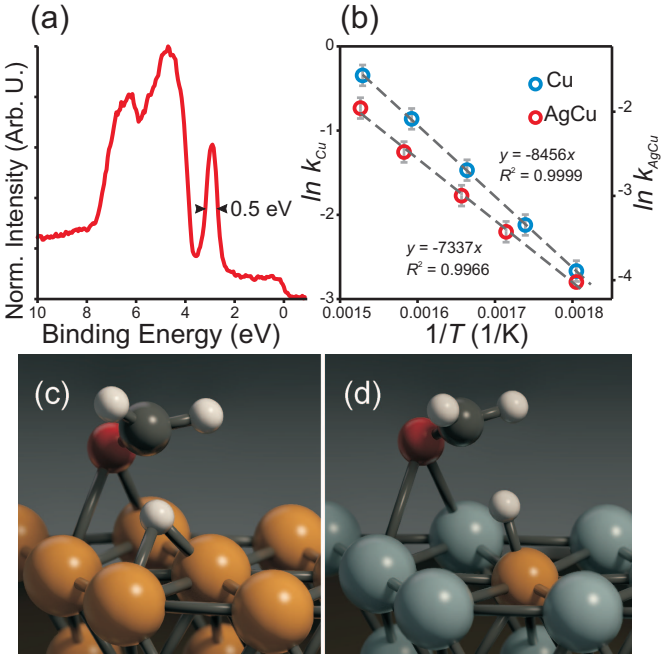

(a)
AgCu
Ag
Normalized Intensity (arb.u.)
Binding Energy (eV)
(b)
AgCu (Difference)
Cu
2.5 eV
0.5 eV
Normalized Intensity (arb.u.)
Binding Energy (eV)
(c)
Cu 4s
Cu 4p
Cu 3d (total)
Cu 3d (t_{2g})
Cu 3d (e_g)
Density of States (arb. u.)
Binding Energy (eV)
(d)
Cu 4s
Cu 4p
Cu 3d (total)
Cu 3d (t_{2g})
Cu 3d (e_g)
Density of States (arb. u.)
Binding Energy (eV)

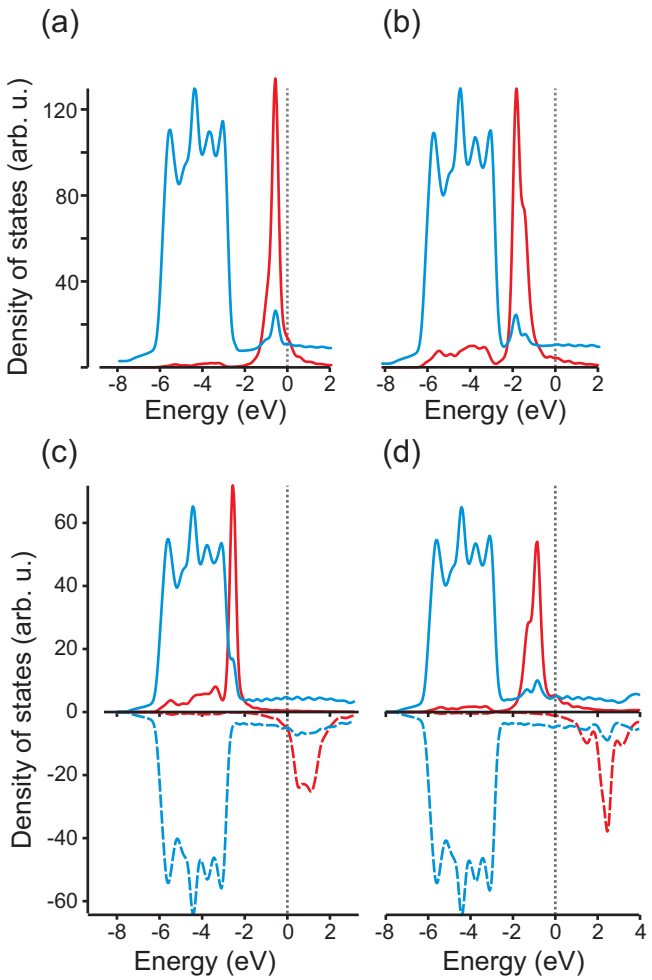

(a)
Cu
AgCu
0.23 eV
Normalized Intensity (Arb. U)
936
932
928
Binding Energy (eV)
(b)
α
β
γ
Bulk Cu
AgCu (0.3%Cu)
Normalized Intensity (Arb. U)
930
935
940
Excitation Energy (eV)
(c)
α
β
γ
Bulk Cu
Ag31Cu1
Normalized Intensity (Arb. U)
930
935
940
Excitation Energy (eV)


(a)
i) Metal interaction on
ii) Metal interaction off
Binding Energy
E_{Fermi}
Adsorbate Orbital
Broadened State
s-Band
(b)
i) Metal interaction on
ii) Metal interaction off
Binding Energy
E_{Fermi}
Anti-bonding
d-Band
Adsorbate Orbital
Bonding
(c)
DOS (arb. u.)
E_{Fermi}
Energy
(d)
DOS (arb. u.)
E_{Fermi}
Energy


(a)
Cu36
O 2p
Cu 3d
Density of States (arb. u.)
σ
nb
σ*
EFermi
-4
-2
0
(b)
Adsorbate
Metal
d-interaction on
d-interaction off
Gas
EFermi
σ*
nb
σ
2px,y
2pz
2px,y,z
Energy
Cu 3d
(c)
px,py
pz
σ*
σ
EFermi
DOS (arb. u.)
Energy
(d)
Ag35Cu1
O 2p
Cu 3d
Density of States (arb. u.)
σ
π
π* σ*
EFermi
-4
-2
0
Energy (eV)
(e)
EFermi
σ*
π*
π
σ
2px,y
2pz
2px,y,z
Energy
Cu 3d
(f)
px,py
pz
π*
σ*
σ
π
EFermi
DOS (arb. u.)
Energy
(g)
σ
π
π*
σ*
O
Ag
Cu


(a)
weaker
bonding
to alloy
stronger
bonding
to alloy
Difference in Adsorption Energy [ε_ad.-ε_Cu] ((eV)
ΔElectronegativity [χ_ad.-χ_Cu] (eV)
0.3
0.2
0.1
-0.1
-0.2
-0.3
-0.4
-4
-3
-2
-1
0
1
2
3
4
5
6


(a)
Norm. Intensity (Arb. U.)
0.5 eV
10
8
6
4
2
0
Binding Energy (eV)
(b)
Cu
AgCu
y = -8456x
R² = 0.9999
y = -7337x
R² = 0.9966
ln k_Cu
ln k_AgCu
0
-1
-2
-3
-2
-3
-4
0.0015
0.0016
0.0017
0.0018
1/T (1/K)
(c)
(d)


(a)
(b)
(c)
(d)
Density of states (arb. u.)
Energy (eV)
120
80
40
60
20
0
-20
-40
-60
-8
-6
-4
-2
0
2
4