Supporting Information
The effect of elastic strains on the adsorption energy of H, O, and OH in transition metals

Carmen Martínez-Alonso[a,b], José Manuel Guevara-Vela[c], Javier LLorca[a,c]

[a] *IMDEA Materials Institute, C/Eric Kandel 2, 28906 - Getafe, Madrid, Spain.*
[b] *Department of Inorganic Chemistry, Complutense University of Madrid, 28040 Madrid, Spain.*
[c] *Department of Materials Science, Polytechnic University of Madrid, E. T. S. de Ingenieros de Caminos, 28040 Madrid, Spain.*

	Ni	Cu	Pd	Ag	Pt	Au	Rh	Ir
a (Å)	3.52	3.63	3.94	4.09	3.96	4.16	3.77	3.87

Table S1: Lattice parameter a for fcc transition metals obtained from DFT calculations. Values are referred in Å.

	Zn	Cd	Co
a (Å)	2.63	3.01	2.49
c (Å)	5.13	5.84	4.04

Table S2: Lattice parameters a and c for hcp transition metals obtained by DFT calculations. Values are referred in Å.

	H		O		OH	
	m	b	m	b	m	b
Ni	0.06	-0.64	0.37	-3.93	0.45	-0.94
Cu	0.14	-0.49	0.59	-3.71	0.67	-1.04
Pd	0.12	-0.68	0.41	-2.64	0.57	0.02
Ag	0.18	-0.12	0.45	-2.08	0.52	-0.08
Pt	0.19	-1.14	0.43	-3.67	0.63	-1.08
Au	0.27	-0.35	0.96	-2.65	0.91	-0.10
Rh	0.10	-0.94	0.15	-3.61	0.21	-0.61
Ir	0.18	-1.18	0.52	-4.93	0.32	-0.67
Co	-0.05	-0.50	0.82	-3.69	0.85	-0.48
Zn	0.30	-0.05	0.46	-3.72	0.40	-0.54
Cd	0.28	0.26	0.20	-2.65	0.15	0.03

Table S3: Values of coefficients m and b in eq. (4) of the main text for each transition metal and adsorbate (either H, O or OH).

Metal	$E_F(A_0)$
Ni	2.15
Cu	1.73
Pd	1.22
Ag	1.48
Pt	3.57
Au	1.74
Rh	4.23
Ir	4.42
Co	0.32
Zn	2.47
Cd	1.96

Table S4: Fermi energies of clean, underformed metallic slabs. Values of energy are referred in eV.

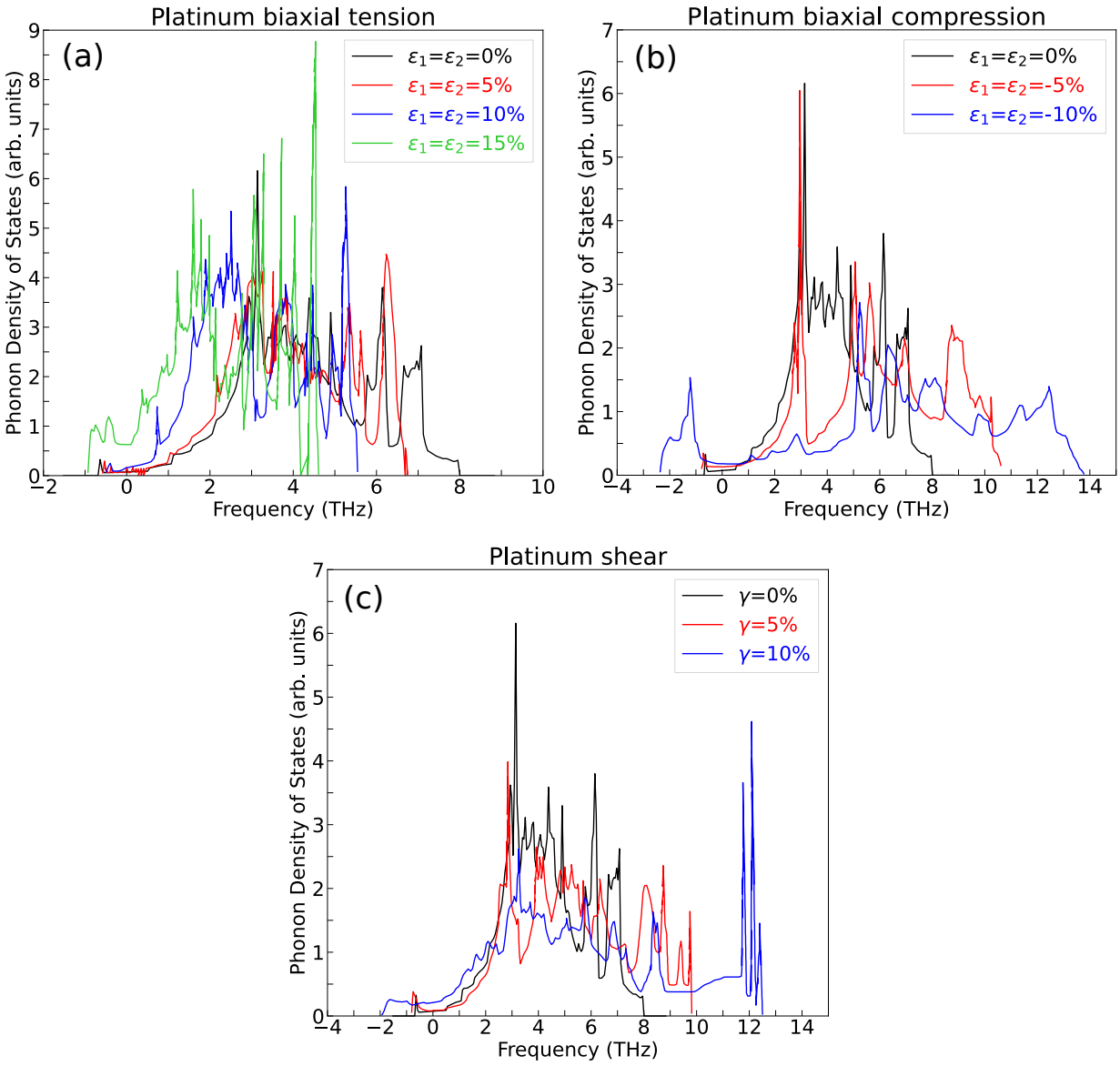

Figure S1: Phonon density of states for the (111) fcc Pt slab subjected to: (a) biaxial tensile strains. (b) Biaxial compressive strains. (c) Shear strains.

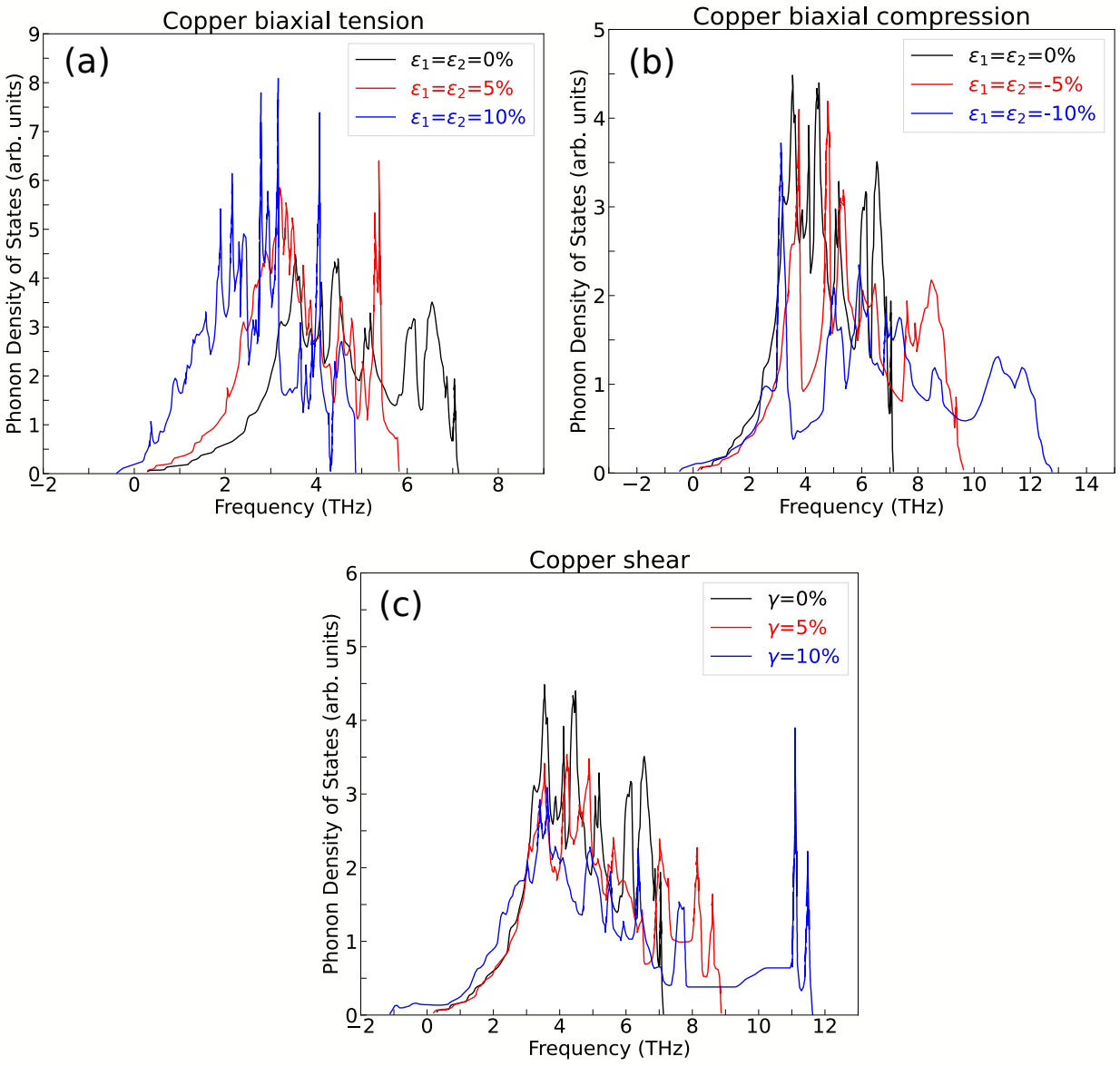

Figure S2: Phonon density of states for the (111) fcc Cu slab subjected to: (a) biaxial tensile strains. (b) Biaxial compressive strains. (c) Shear strains.

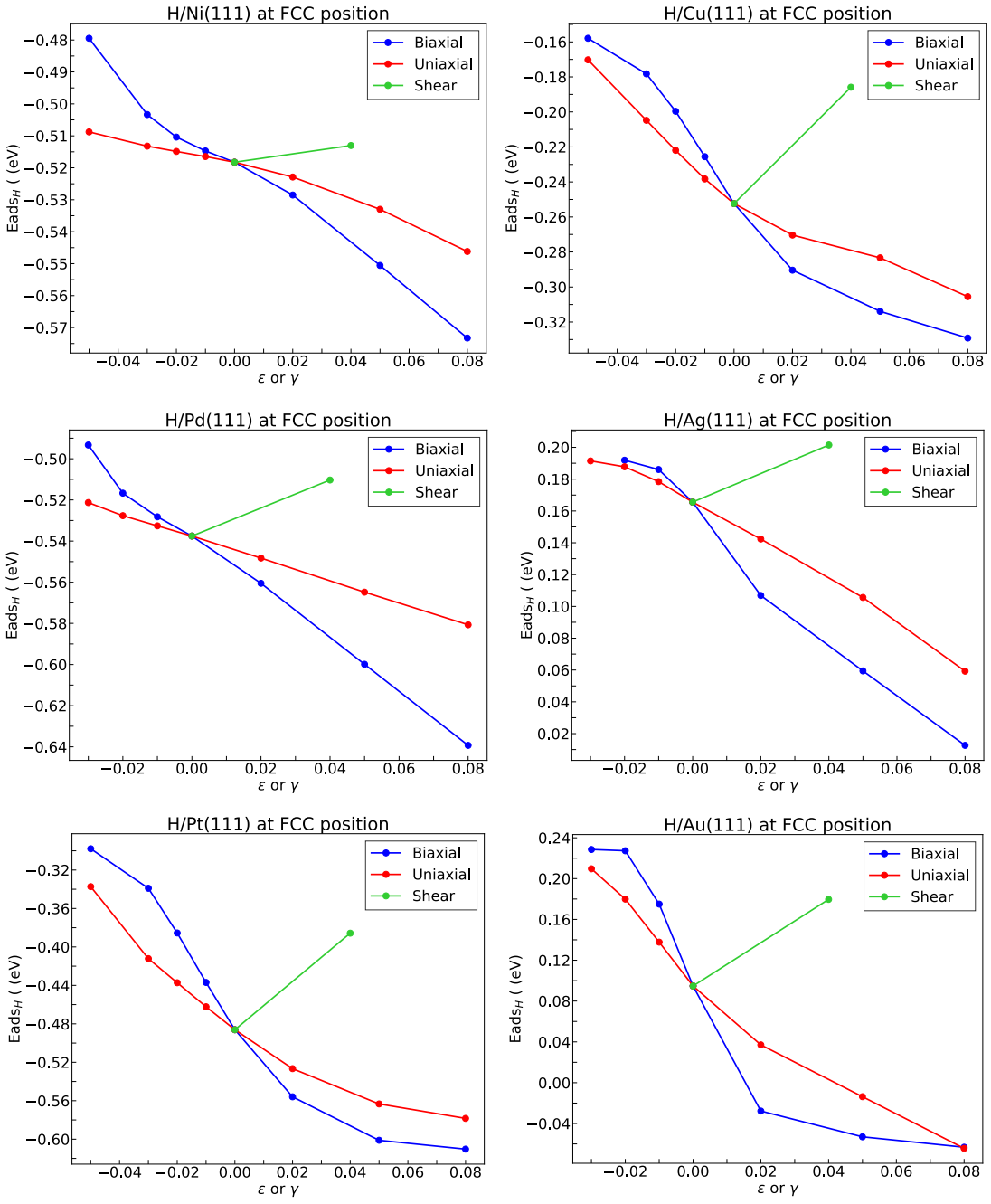

Figure S3: Adsorption energy of H as a function of strain from 5% compression to 8% tension at FCC positions for Ni, Cu, Pd, Ag, Pt, and Au. The legend indicates the type of strain.

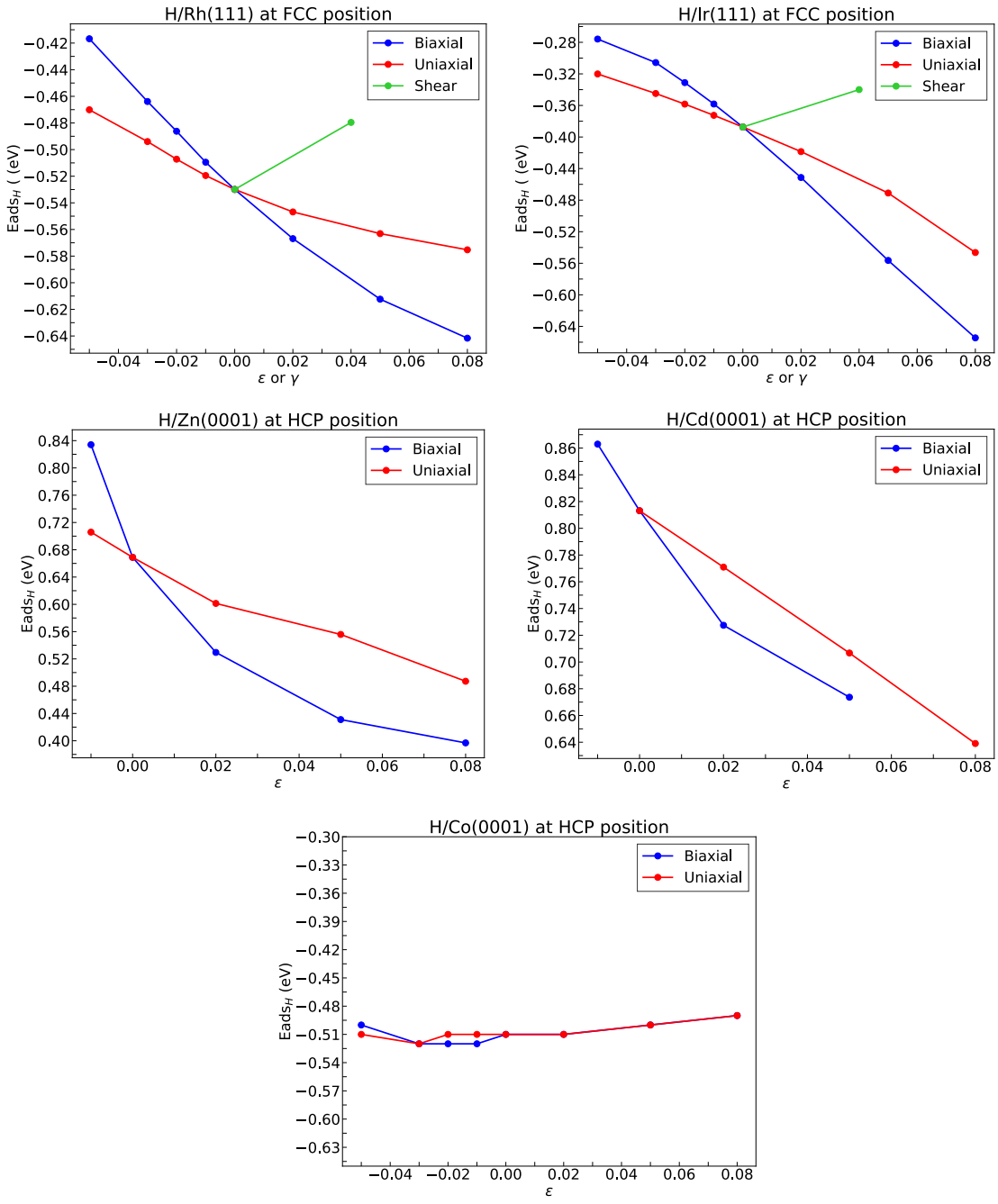

Figure S4: Adsorption energy of H as a function of strain from 5% compression to 8% tension at FCC positions for Rh, and Ir, and HCP position for Zn, Cd, and Co. The legend indicates the type of strain.

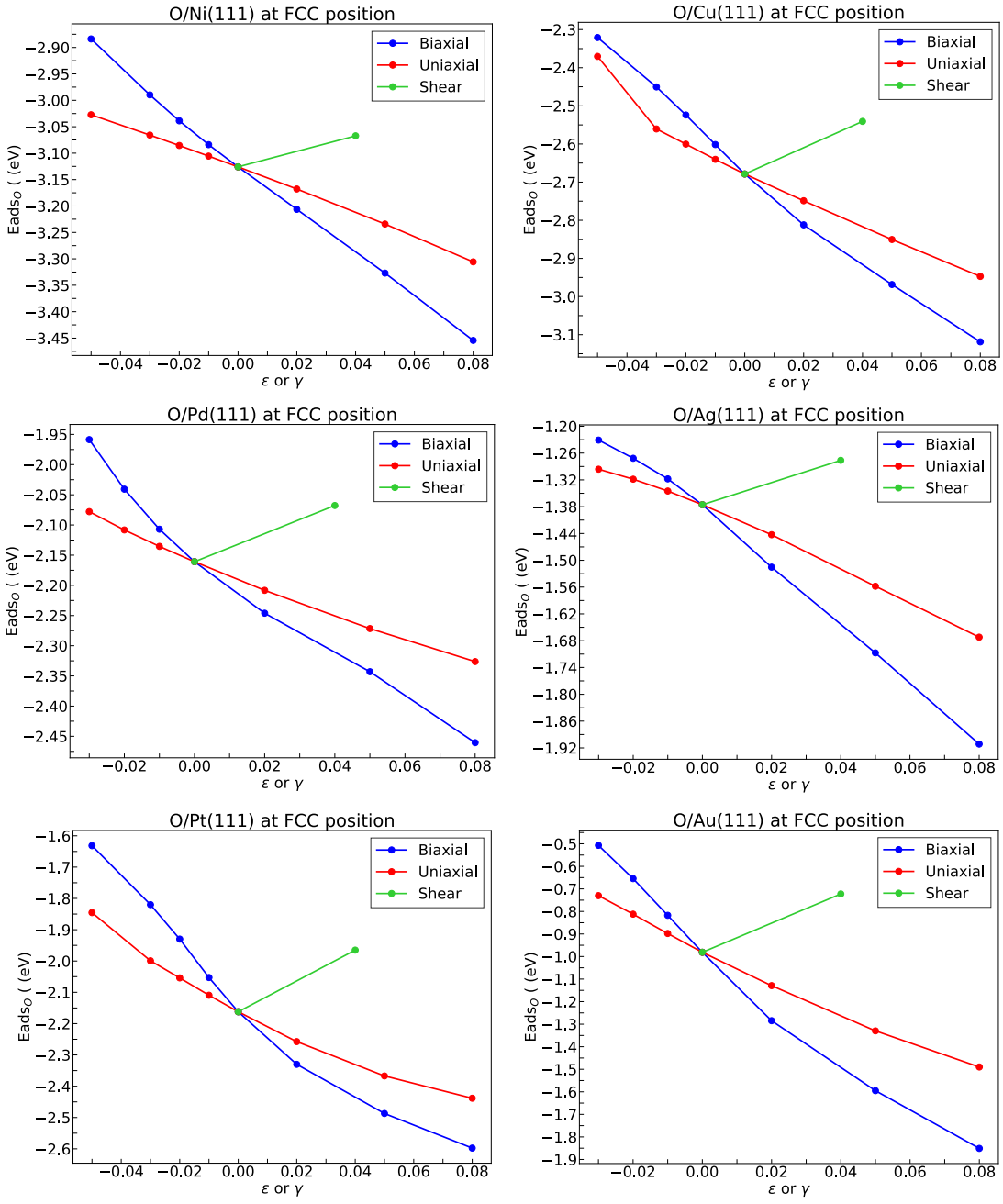

Figure S5: Adsorption energy of O as a function of strain from 5% compression to 8% tension at FCC positions for Ni, Cu, Pd, Ag, Pt, and Au. The legend indicates the type of strain.

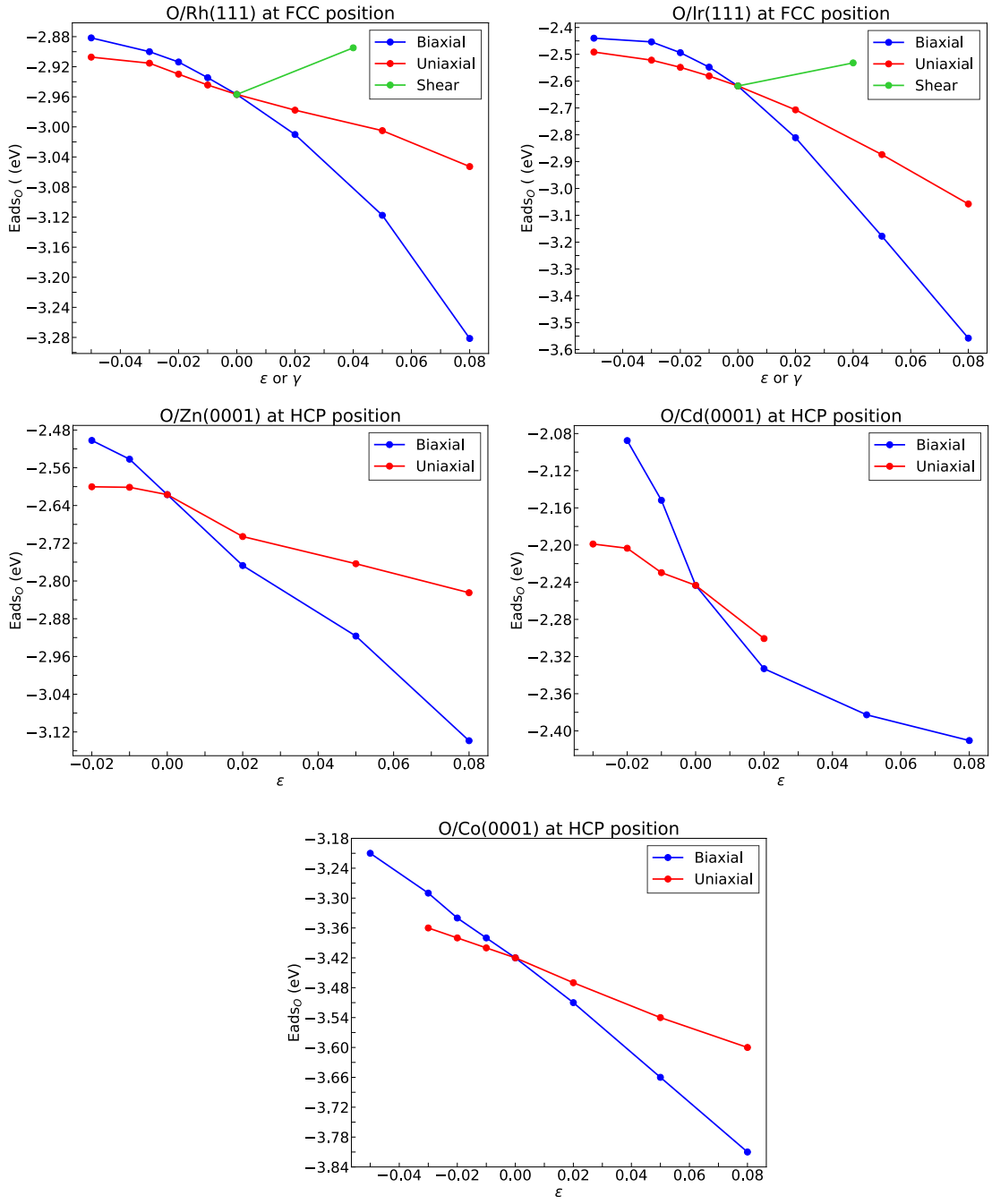

Figure S6: Adsorption energy of O as a function of strain from 5% compression to 8% tension at FCC positions for Rh, and Ir, and HCP positions for Zn, Cd, and Co. The legend indicates the type of strain.

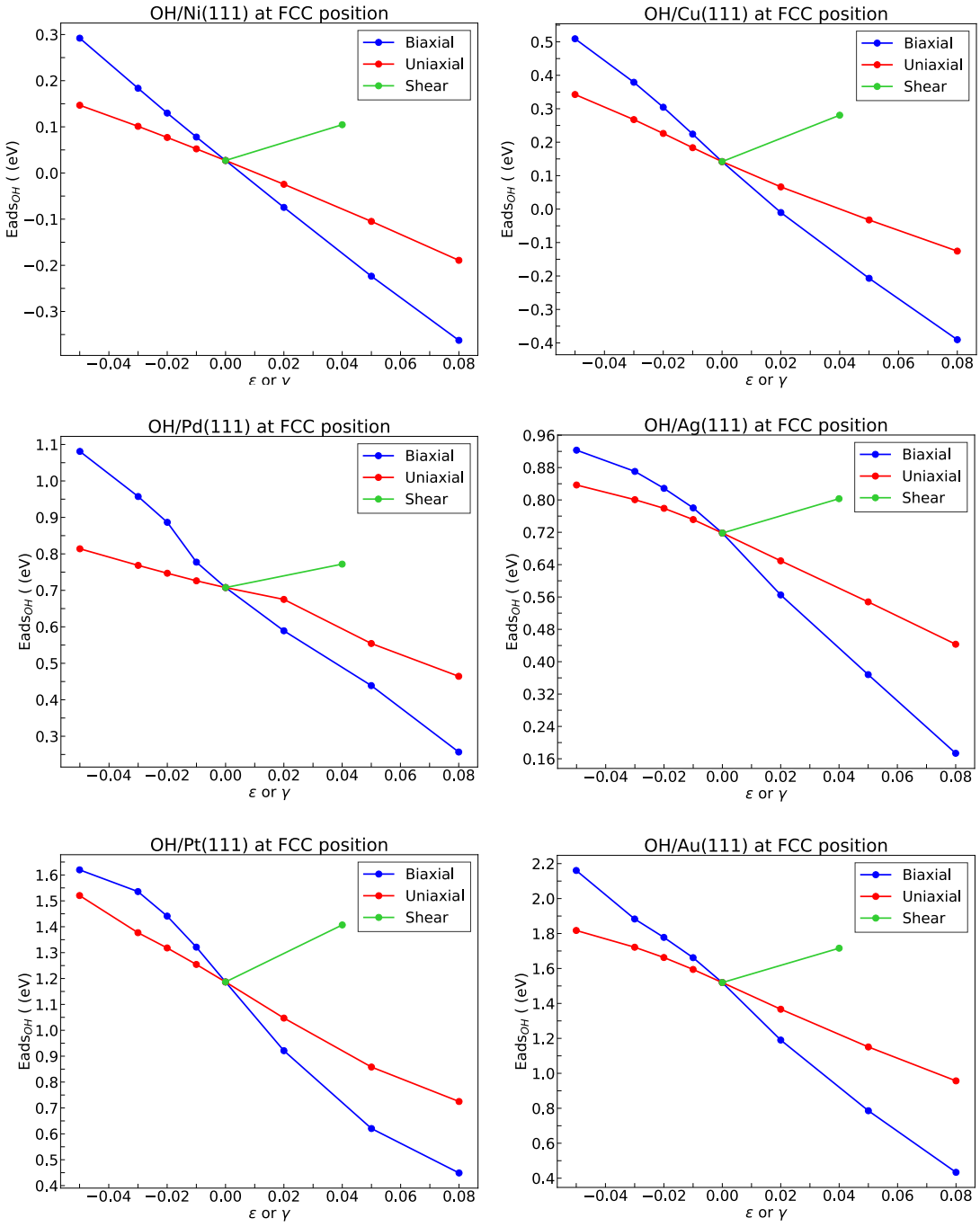

Figure S7: Adsorption energy of OH as a function of strain from 5% compression to 8% tension at FCC positions for Ni, Cu, Pd, Ag, Pt, and Au. The legend indicates the type of strain.

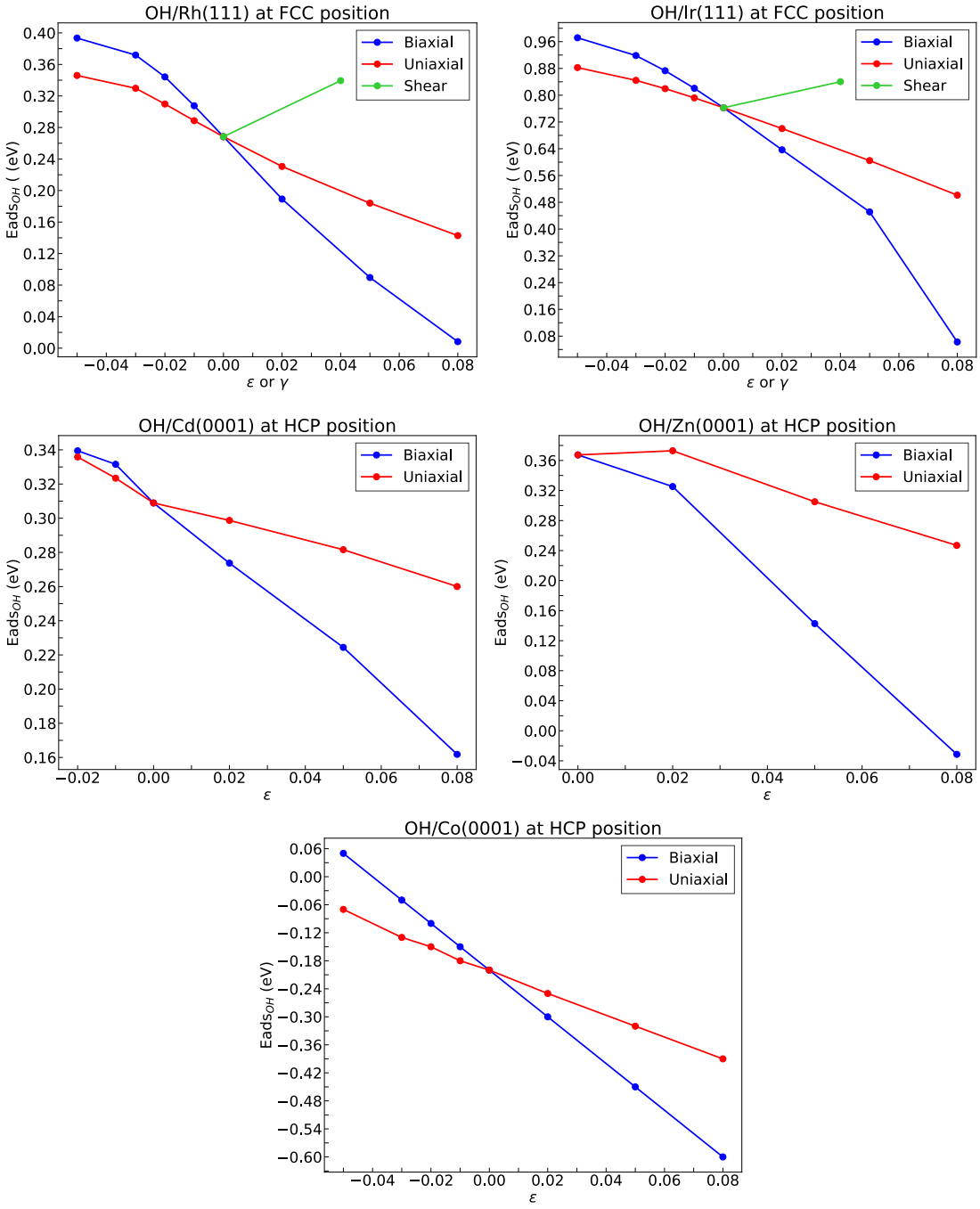

Figure S8: Adsorption energy of OH as a function of strain from 5% compression to 8% tension at FCC positions for Rh, and Ir, and HCP positions for Zn, Cd, and Co. The legend indicates the type of strain.

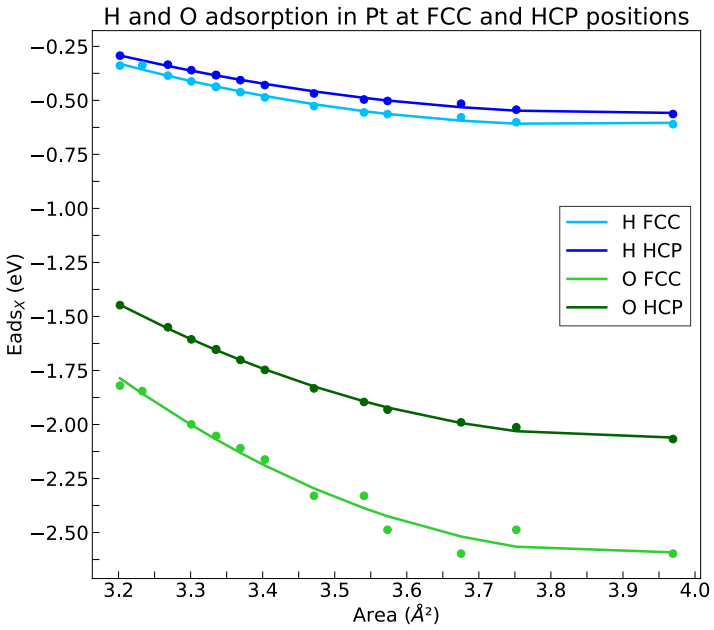

Figure S9: Adsorption energy of H and O in platinum as a function of the area of the FCC and the HCP sites from 5% compression to 8% tension. Dots represent the DFT calculations and lines show the quadratic fittings.