Supplementary Information

First-principle calculations on $CuInSe_2$/AlP heterostructures

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Table S1. AlP(001) surface relaxation of the two types of terminations as a function of the number of layers N in the slab, Δd_{ij} is the change of interlayer distance in the percentage of bulk spacing.

Termination	Change in interlayer	Number of layers N in the slab						
		5(%)	9(%)	13(%)	17(%)	21(%)	25(%)	29(%)
Al-	Δd_{12}	4.93	5.42	4.72	4.54	4.16	3.98	3.88
	Δd_{23}	4.94	2.72	2.15	1.94	1.62	1.44	1.37
	Δd_{34}		1.41	0.87	0.63	0.28	0.17	0.07
	Δd_{45}		1.87	1.08	0.80	0.56	0.35	0.27
	Δd_{56}			1.40	1.12	0.84	0.74	0.62
	Δd_{67}			1.26	1.04	0.84	0.63	0.54
	Δd_{78}				1.04	0.84	0.67	0.58
	Δd_{89}				1.02	0.94	0.74	0.62
	Δd_{910}					0.87	0.74	0.62
	Δd_{1011}					0.87	0.74	0.66
	Δd_{1112}						0.74	0.66
	Δd_{1213}						0.77	0.66
								0.70
								0.66
P-	Δd_{12}	-1.11	-1.75	-1.49	-3.18	-2.28	-2.38	-2.52
	Δd_{23}	3.18	3.28	3.30	3.16	3.09	3.02	2.99
	Δd_{34}		0.11	-0.96	-1.37	-1.51	-1.65	-1.70
	Δd_{45}		1.65	1.81	1.64	1.54	1.47	1.43
	Δd_{56}			0.47	0.10	-0.05	-0.14	-0.17
	Δd_{67}			0.89	0.77	0.67	0.56	0.53
	Δd_{78}				0.39	0.23	0.14	0.10
	Δd_{89}				0.56	0.51	0.42	0.33
	Δd_{910}					0.36	0.25	0.18
	Δd_{1011}					0.42	0.35	0.29
	Δd_{1112}						0.28	0.25
	Δd_{1213}						0.32	0.25
								0.25
								0.25

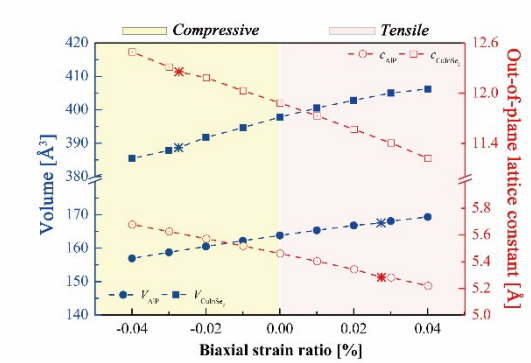

Figure S1. Calculation of the conventional cells in out-of-plane lattice constant and volume of AlP and $CuInSe_2$ as a function of biaxial strain ratio in [-4%;4%].

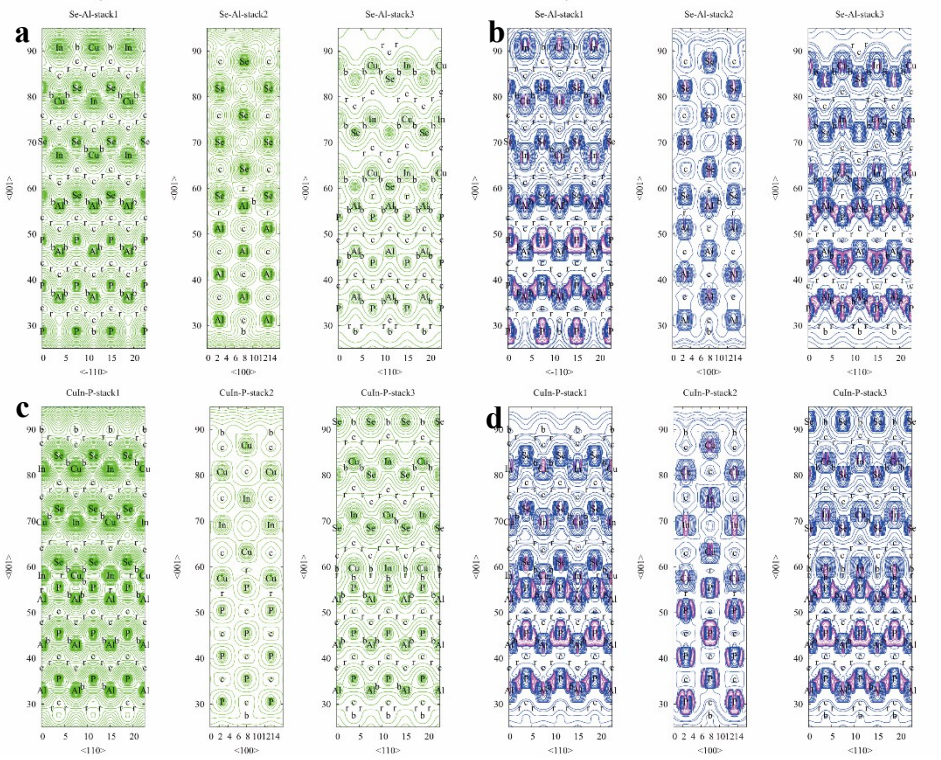

Figure S2. Topological properties of Se-Al terminated and Cu/In-P terminated heterostructure: electron density (a and c) and electron density Laplacian (b and d).