Supporting Information: The structural and electronic richness of buckled honeycomb AsP bilayers

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Table S1. The lattice constant, a, buckling height, Δz, and interlayer distance, d, as well as the relative energies computed with different levels of theory (including ZPE correction) for the sixteen stacking configurations of blue AsP.

		PBE+MBD				SCAN+rVV10				PBE0+DDsC		ACFDT-RPA+PBE0
	Configuration	***a***	**Δ*z***	***d***	**Δ*E***	***a***	**Δ*z***	***d***	**Δ*E***	***d***	**Δ*E***	**Δ*E***
Group I	$A_{-1}A'_{-1}$	3.44	1.32	4.53	42.4	3.42	1.30	4.62	4.4	4.58	0.8	0.0
	A_1A_1	3.44	1.32	4.61	41.5	3.42	1.30	4.67	4.1	4.62	0.0	
	$A_1A'_1$	3.44	1.32	4.70	41.8	3.42	1.30	4.90	4.9	4.70	0.2	
	A'_1B_1	3.45	1.32	4.36	41.6	3.42	1.30	4.69	5.3	4.59	2.7	
	$A'_1B'_1$	3.45	1.32	4.54	41.7	3.42	1.30	4.72	5.3	4.71	2.3	
	A_1B_1	3.45	1.32	4.47	41.0	3.42	1.30	4.67	4.7	4.75	1.8	
	$A_1B'_1$	3.45	1.32	4.66	42.2	3.42	1.30	4.81	5.7	4.78	2.5	
	A_1B_{-1}	3.45	1.32	4.88	46.2	3.42	1.30	4.92	9.0	4.88	5.0	
Group II	$A'_{-1}B_1$	3.44	1.32	5.40	53.2	3.41	1.30	5.36	17.2	5.51	12.5	14.8
	$A_{-1}B_1$	3.44	1.32	5.37	54.2	3.41	1.30	5.54	18.9	5.30	12.9	
	$A_1A'_{-1}$	3.44	1.32	5.46	53.8	3.41	1.31	5.45	17.9	5.45	12.5	
	$A'_{-1}B'_1$	3.44	1.32	5.45	53.0	3.41	1.30	5.50	17.0	5.51	11.9	
	$A'_1A'_{-1}$	3.44	1.32	5.43	54.8	3.41	1.30	5.41	18.6	5.43	12.7	
	A_1A_{-1}	3.44	1.32	5.49	53.6	3.41	1.31	5.59	17.6	5.50	11.9	
Group II	$A'_1B'_{-1}$	3.53	1.28	3.07	0.0	3.51	1.25	3.13	0.0	3.11	9.5	24.5
	$A_1B'_{-1}$	3.55	1.26	3.34	40.5	3.52	1.25	3.39	29.2	3.52	38.4	
	Monolayer	3.44	1.32	-	-	3.42	1.30	-	-	-	-	

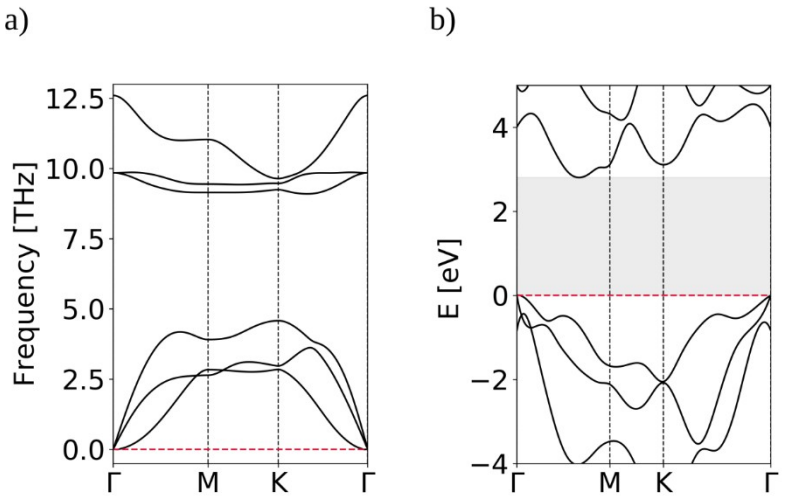

Figure S1. a) The phonon and b) electronic band structure within G_0W_0 of the blue AsP monolayer.

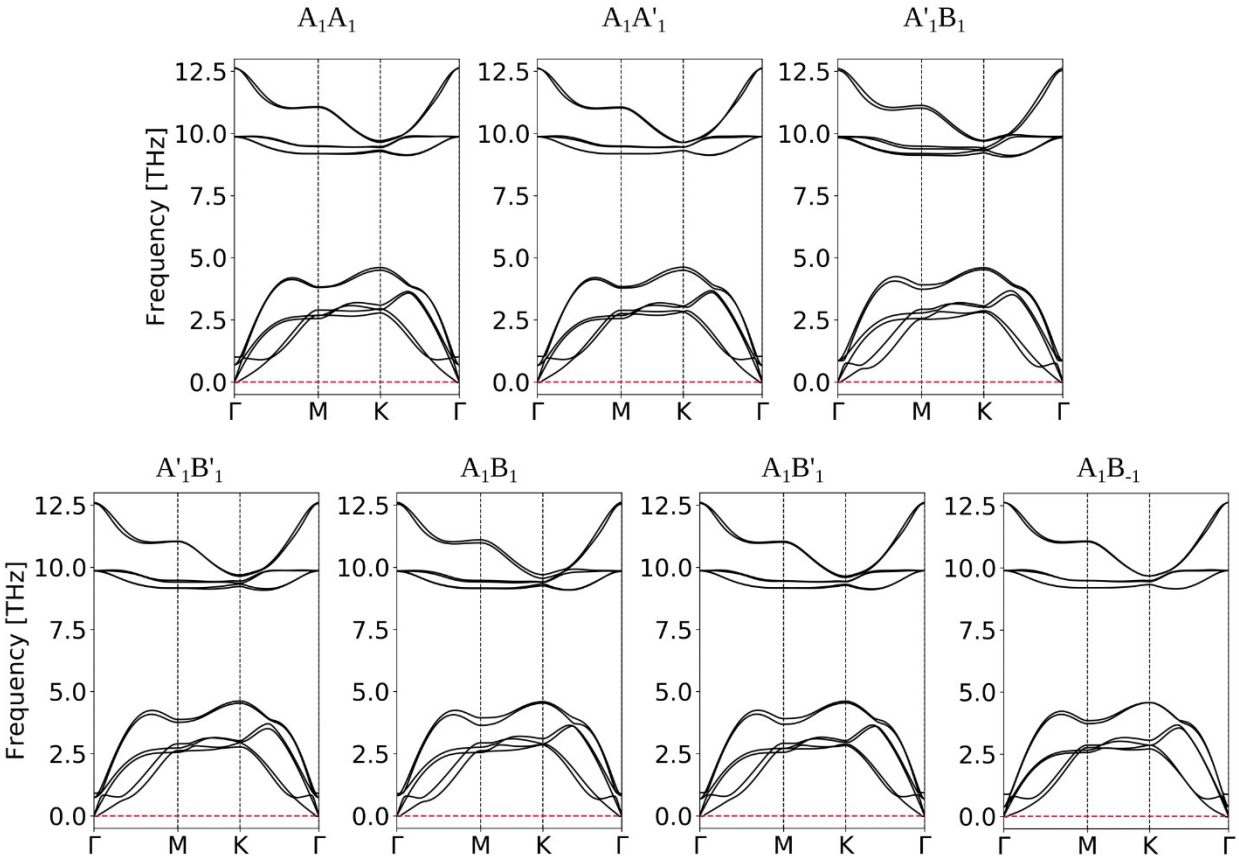

Figure S2. The phonon structures of bilayers of group I.

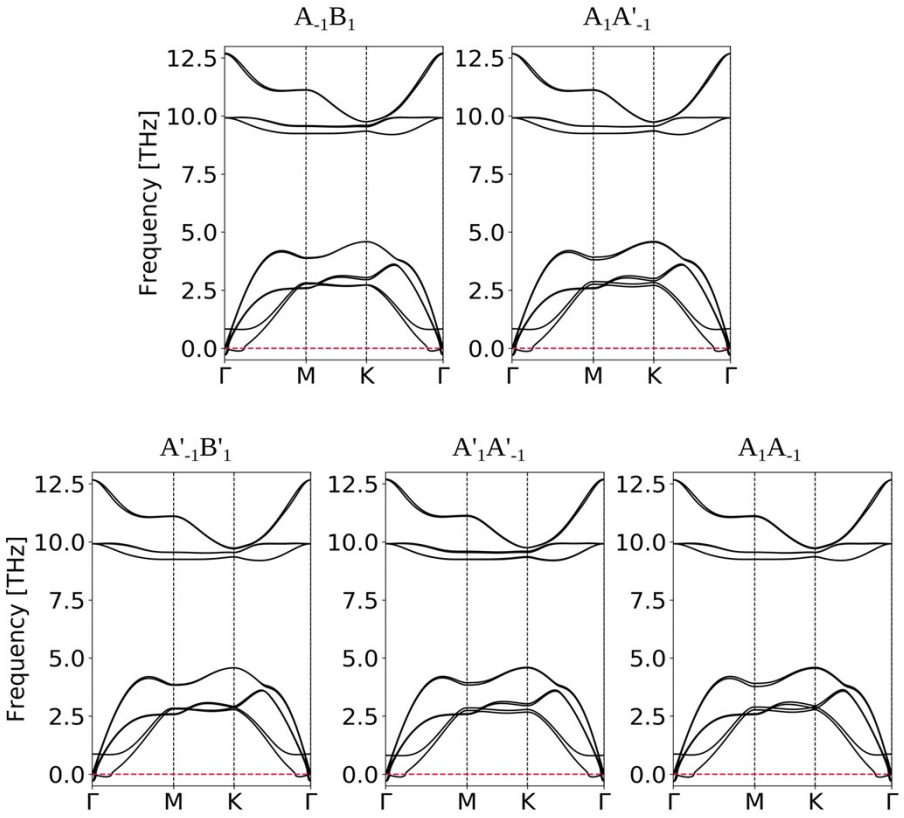

Figure S3. The phonon structures of bilayers of group II.

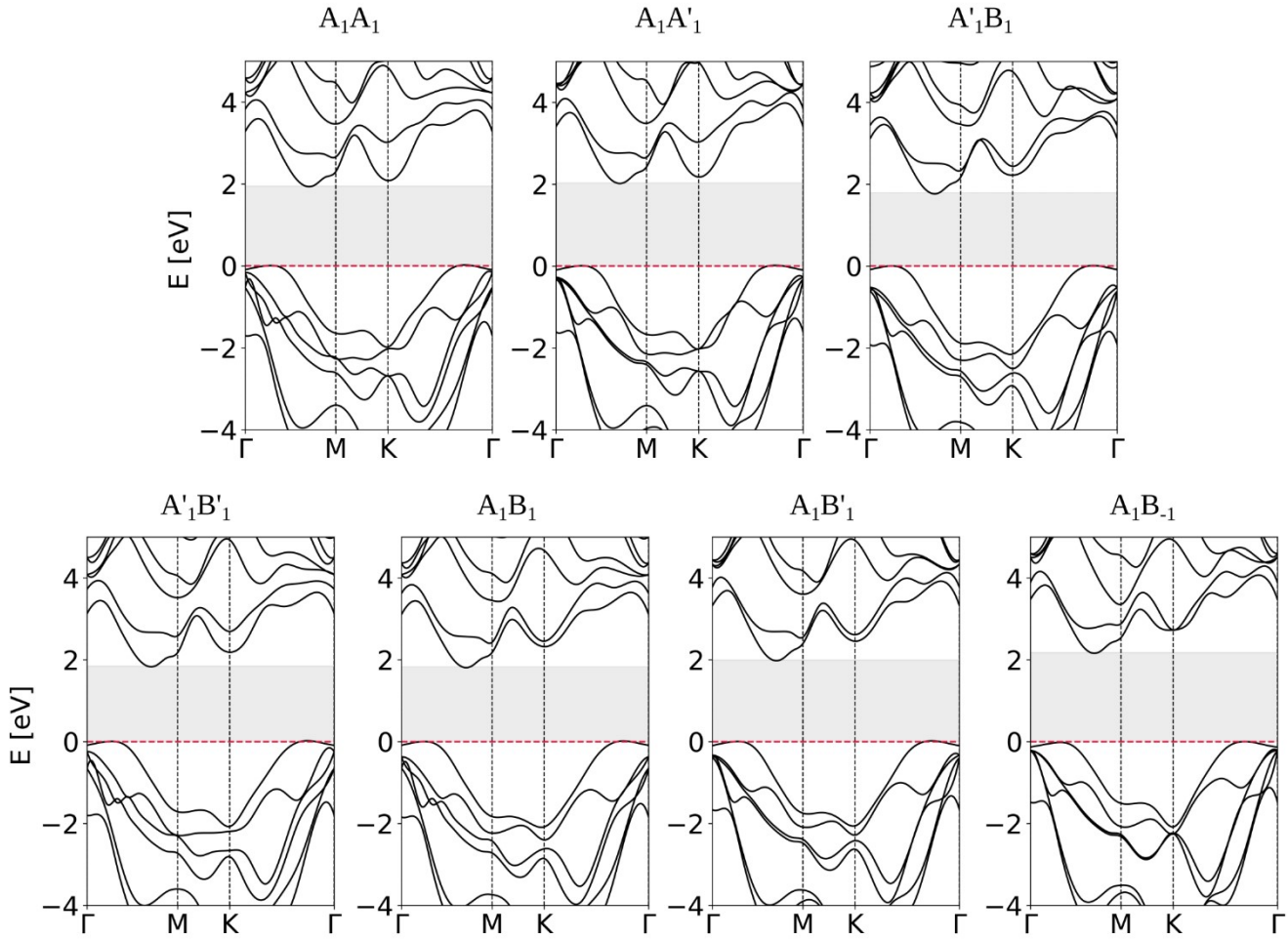

Figure S4. The G_0W_0 electronic band structures of bilayers of group I.

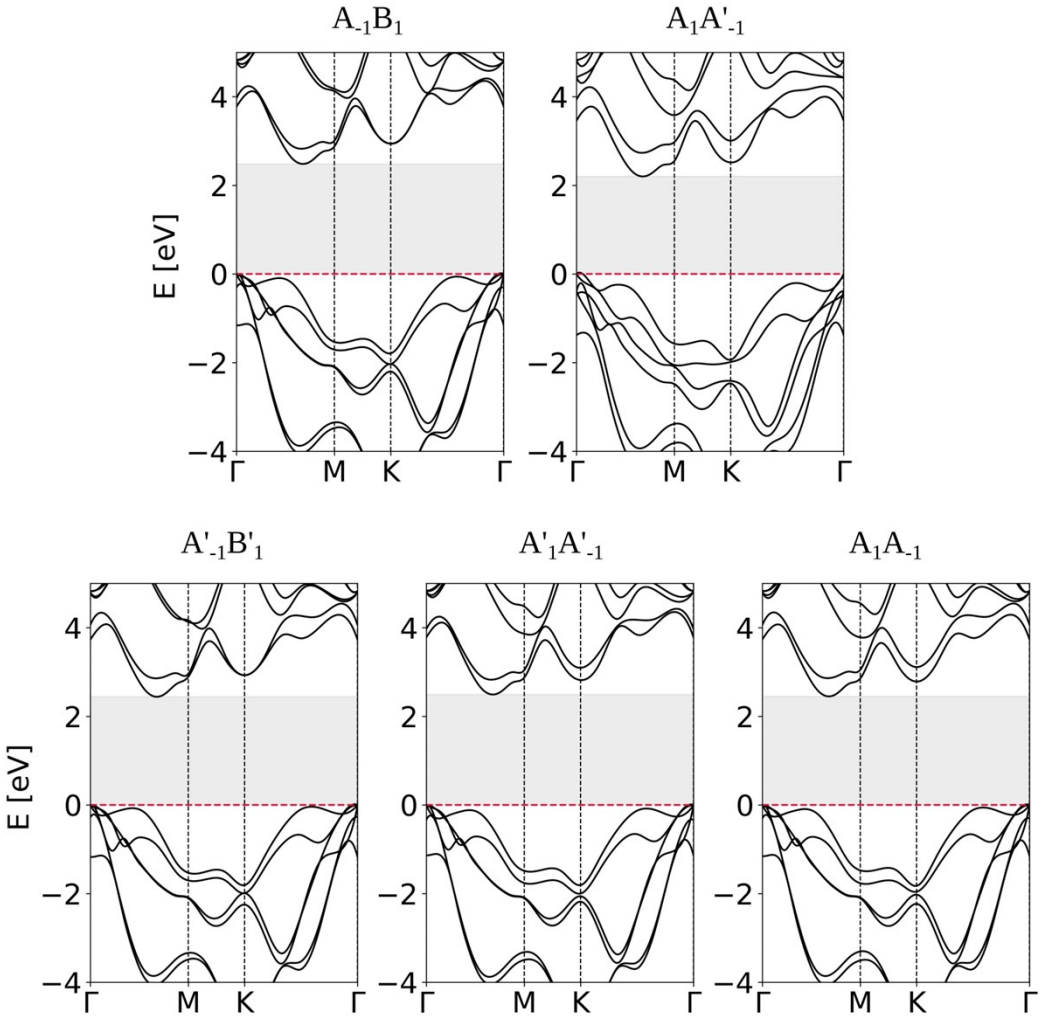

Figure S5. The G_0W_0 electronic band structures of bilayers of group II.

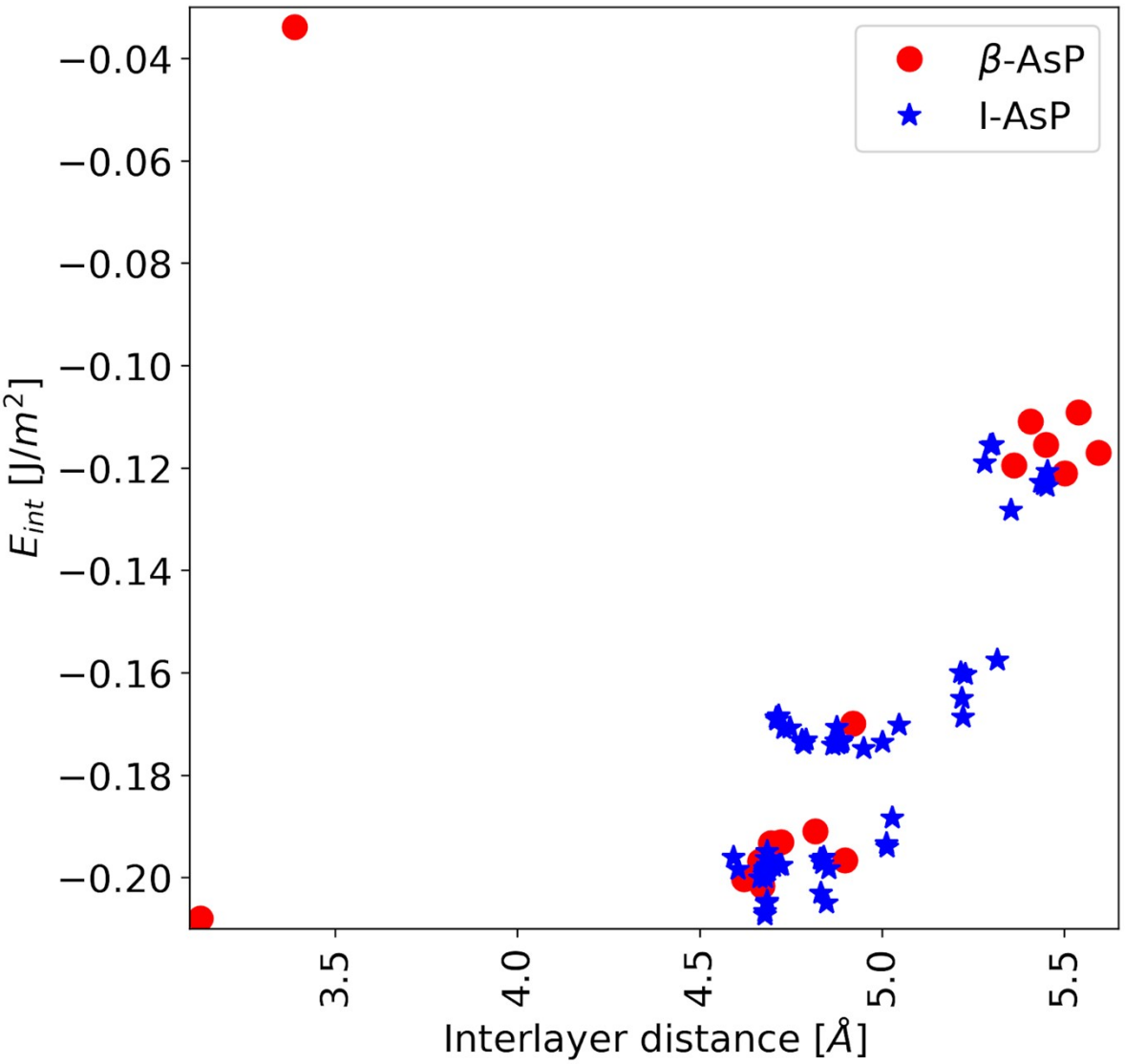

Figure S6. Interlayer interaction energies per area as a function of the interlayer distance for β- and I-AsP bilayers.

Classical dipole-dipole energy definition

$$E_{dip-dip} = -\frac{p_1 p_2 3cos\alpha cos\theta - cos\beta}{4\pi\epsilon_0 \quad r^3}$$

p_1, p_2: dipoles of upper and bottom layers, respectively.

r: the interlayer distance or the distance between p_1 and p_2.

α, θ: angles between p_1 and r and between p_2 and r, respectively.

β: angle between p_1 and p_2.