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Novel Electronic Properties of Two-Dimensional As_xSb_y Alloys Studied by Using DFT

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Fig. S1 Optimized monolayer configurations of (a) α-$As_{18}Sb_{18}$ and (b) β-$As_{18}Sb_{18}$.

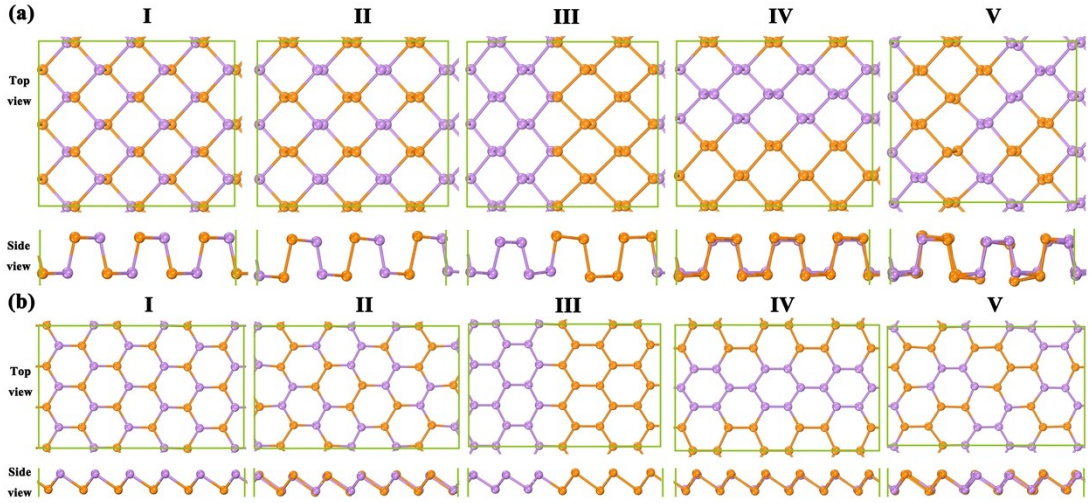

Fig. S2 (a) Electronic band gaps of As_xSb_y monolayer calculated by PBE and HSE06 approaches. Electronic band structures of As_8Sb_8 in α phase (b) and β phase (c) calculated by PBE and HSE06.

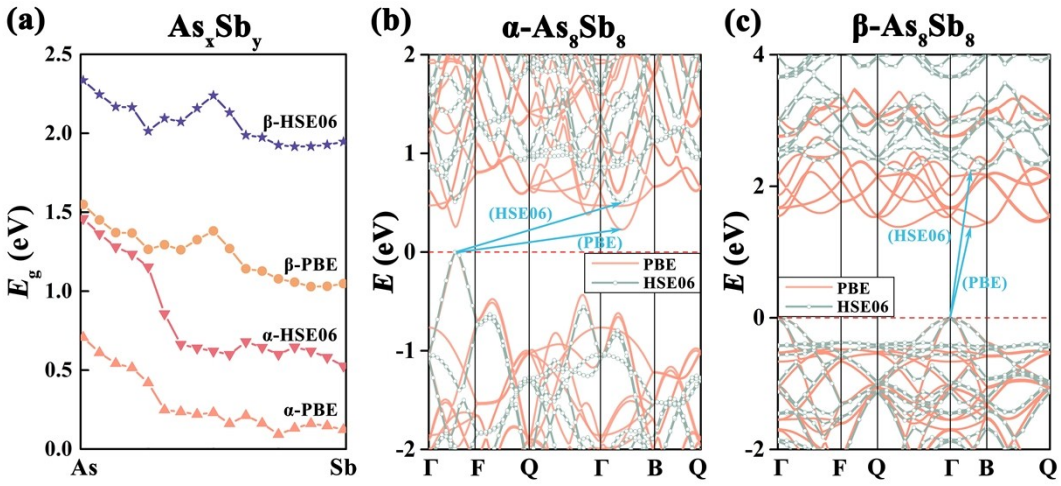

Table S1: The lattice constants of relaxed configurations for As_xSb_y monolayer alloys.

	α-phase		β-phase	
As	a_1=9.36, a_2=7.29		a_1=12.40, a_2=7.16	
$As_{15}Sb_1$	a_1= 9.35, a_2=7.37		a_1=12.49, a_2=7.21	
$As_{14}Sb_2$	I: a_1=9.31, a_2=7.47	II: a_1=9.36, a_2=7.46	I: a_1=12.59, a_2=7.27	II: a_1=12.59, a_2=7.26
$As_{13}Sb_3$	I: a_1=9.31, a_2=7.55	II: a_1=9.41, a_2=7.53	I: a_1=12.69, a_2=7.34	II: a_1=12.69, a_2=7.34
	III: a_1=9.37, a_2=7.54	IV: a_1=9.33, a_2=7.54	III: a_1=12.70, a_2=7.33	IV: a_1=12.69, a_2=7.34
$As_{12}Sb_4$	I: a_1=9.11, a_2=7.67	II: a_1=9.32, a_2=7.63	I: a_1=12.80, a_2=7.40	II: a_1=12.78, a_2=7.39
	III: a_1=9.24, a_2=7.64	IV: a_1=9.35, a_2=7.63	III: a_1=12.76, a_2=7.39	IV: a_1=12.74, a_2=7.41
$As_{11}Sb_5$	I: a_1=9.39, a_2=7.70	II: a_1=9.04, a_2=7.77	I: a_1=12.91, a_2=7.46	II: a_1=12.92, a_2=7.46
	III: a_1=9.10, a_2=7.75	IV: a_1=9.42, a_2=7.70	III: a_1=12.89, a_2=7.46	IV: a_1=12.85, a_2=7.46
$As_{10}Sb_6$	I: a_1=8.79, a_2=7.89	II: a_1=8.76, a_2=7.90	I: a_1=13.03, a_2=7.52	II: a_1=13.03, a_2=7.52
	III: a_1=9.37, a_2=7.80	IV: a_1=9.39, a_2=7.79	III: a_1=12.98, a_2=7.52	IV: a_1=12.95, a_2=7.52
As_9Sb_7	I: a_1=8.77, a_2=7.97	II: a_1=9.42, a_2=7.87	I: a_1=13.14, a_2=7.59	II: a_1=13.14, a_2=7.59
	III: a_1=9.43, a_2=7.86	IV: a_1=9.31, a_2=7.89	III: a_1=13.10, a_2=7.57	IV: a_1=13.03, a_2=7.58
As_8Sb_8	I: a_1=8.75, a_2=8.04	II: a_1=9.19, a_2=7.97	I: a_1=13.24, a_2=7.65	II: a_1=13.23, a_2=7.62
	III: a_1=9.10, a_2=8.01	IV: a_1=9.09, a_2=8.02	III: a_1=13.15, a_2=7.64	IV: a_1=13.11, a_2=7.64
As_7Sb_9	I: a_1=9.40, a_2=8.03	II: a_1=9.43, a_2=8.03	I: a_1=13.33, a_2=7.70	II: a_1=13.33, a_2=7.70
	III: a_1=9.42, a_2=8.02	IV: a_1=9.10, a_2=8.09	III: a_1=13.28, a_2=7.69	IV: a_1=13.23, a_2=7.70
As_6Sb_{10}	I: a_1=8.93, a_2=8.17	II: a_1=9.07, a_2=8.15	I: a_1=13.40, a_2=7.70	II: a_1=13.42, a_2=7.74
	III: a_1=8.94, a_2=8.15	IV: a_1=9.12, a_2=8.17	III: a_1=13.38, a_2=7.75	IV: a_1=13.35, a_2=7.75
As_5Sb_{11}	I: a_1=9.21, a_2=8.19	II: a_1=9.30, a_2=8.20	I: a_1=13.50, a_2=7.80	II: a_1=13.51, a_2=7.80
	III: a_1=9.02, a_2=8.22	IV: a_1=9.01, a_2=8.24	III: a_1=13.48, a_2=7.81	IV: a_1=13.45, a_2=7.80
As_4Sb_{12}	I: a_1=9.24, a_2=8.26	II: a_1=9.20, a_2=8.29	I: a_1=13.58, a_2=7.86	II: a_1=13.56, a_2=7.86
	III: a_1=9.30, a_2=8.27	IV: a_1=9.13, a_2=8.31	III: a_1=13.55, a_2=7.85	IV: a_1=13.55, a_2=7.86
As_3Sb_{13}	I: a_1=9.21, a_2=8.34	II: a_1=9.29, a_2=8.33	I: a_1=13.69, a_2=7.90	II: a_1=13.67, a_2=7.91
	III: a_1=9.16, a_2=8.37	IV: a_1=9.23, a_2=8.35	III: a_1=13.68, a_2=7.91	IV: a_1=13.68, a_2=7.91
As_2Sb_{14}	I: a_1=9.23, a_2=8.43	II: a_1=9.25, a_2=8.41	I: a_1=13.78, a_2=7.95	II: a_1=13.78, a_2=7.96
As_1Sb_{15}	a_1=9.29, a_2=8.48		a_1=13.87, a_2=8.01	
Sb	a_1=9.24, a_2=8.56		a_1=13.96, a_2=8.06	