Supporting Information

New Manifold Two-dimensional Single-layer Structure of Zinc-blende Compounds

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Table SI. Calculated Bader charges of 38 stable free-standing and one unstable (red color) 2D single-layer MX structures. The unit is elementary charge （e）. All the results are calculated by using PBE functional.

H		V		T	
BN	2.06	AlP	1.80	BN	2.12
BP	0.23	GaP	0.74	AlN	2.37
BAs	0.26	GaAs	0.52	AlP	2.20
BSb	0.55	GaSb	0.22	AlAs	1.80
AlN	2.26	InP	0.71	AlSb	1.31
GaN	1.38	InAs	0.57	ZnO	1.22
InN	1.30	InSb	0.27	ZnS	0.86
ZnO	1.05	ZnS	0.83	ZnSe	0.70
BeO	1.68	ZnSe	0.67	ZnTe	0.47
—	—	ZnTe	0.45	CdS	0.84
—	—	CdS	0.75	CdSe	0.70
—	—	CdSe	0.62	CdTe	0.50
—	—	CdTe	0.43	BeO	1.70
—	—	BeS	1.53	BeS	1.54
—	—	—	—	BeSe	1.46
—	—	—	—	BeTe	1.30