Supplementary Information

A novel interstitial site in binary rock-salt compounds

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Materials	Defects	Formation energy (eV) (3x3x3)	Formation energy (eV) (4x4x4)
KCl	Cl- body interstitial	1.74	1.75
	Cl- base interstitial	1.32	1.31
	Split <111>	1.41	1.40
	Split <110>	1.32	1.32
PbS	S- body interstitial	3.01	3.06
	S- base interstitial	1.68	1.69
	S- vacancy	2.05	2.05
	Split <111>	1.45	1.43
	Split <110>	1.49	1.52
AgBr	Br- Split <111>	1.31	1.36

Table S1. Defect formation energy (eV) of selected defects with supercell size. The formation energies are converged to better than 0.05 eV with the supercell size.

Materials	Defects	Formation energy (eV) (3x3x3)
KCl	K- body interstitial	0
	K- base interstitial	0.2
KBr	K- body interstitial	0
	K- base interstitial	0.2
PbS	Pb- body interstitial	0
	Pb- base interstitial	0.40
AgCl	Ag- body interstitial	0
	Ag- base interstitial	0.06

Table S2. Defect formation energy (eV) of cation interstitials in selected rock salt materials. Defect formation energy of the most stable interstitial configuration (body interstitial) is set to zero.

Materials	**Defects**	**Most displaced atom**	**Displacements (Å)**
PbS	Body	S	0.40
	Base	Pb	0.58
	Split <111>	Pb	0.38
	Split <110>	Pb	0.43
PbSe	Body	Se	0.37
	Base	Pb	0.64
	Split <111>	Pb	0.45
	Split <110>	Pb	0.49
CaS	Body	S	0.36
	Base	Ca	0.52
	Split <111>	Ca	0.37
	Split <110>	Ca	0.44
MgSe	Body	Se	0.54
	Base	Se	0.63
	Split <111>	Mg	0.52
	Split <110>	Mg	0.53
KCl	Body	Cl	0.42
	Base	K	0.61

	Split <111>	K	0.32
	Split <110>	K	0.50
KBr	Body	Br	0.48
	Base	Br	0.69
	Split <111>	K	0.37
	Split <110>	K	0.54
AgCl	Body	Cl	0.69
	Base	Cl	0.99
	Split <111>	Cl	1.02
	Split <110>	Ag	1.20
AgBr	Body	Br	0.71
	Base	Br	0.98
	Split <111>	Br	0.99
	Split <110>	Ag	0.83

Table S3. Displacement (in Å) of the nearest-neighboring atoms from their original positions in the defect-bearing supercells. The most displaced configuration in each system is marked in bold.