

Supplemental Material for: Emergence of superconductivity by intercalation of alkali metals and alkaline earth metals in Janus transition-metal dichalcogenides heterostructures

Soukaina Er-Rahmany^{a,b,*}, Mohammed Loulidi^{a,*}, Abdallah El Kenz^a, Abdelilah Benyoussef^{a,c}, Mohamed Balli^b, Mohamed Azzouz^d

^a*Laboratory of Condensed Matter and Interdisciplinary Sciences, Unite de Recherche Labellisee CNRST, URL-CNRST-17, Faculty of Sciences, Mohammed V University of Rabat, Morocco.*

^b*AMEEC Team, LERMA, College of Engineering and Architecture, International University of Rabat, Parc Technopolis, Rocade de Rabat-Salé, 11100, Morocco.*

^c*Hassan II Academy of Sciences and Techniques, Rabat, Morocco.*

^d*Al Akhawayn University, School of Science and Engineering, P.O Box 104, Hassan II Avenue, 53000 Ifrane, Morocco*

*Correspondence author: errahmanysoukaina@gmail.com,
soukainaerrahmany@um5.ac.ma
loulidim60@gmail.com

Table.S1The convergence tests for the electron-phonon coupling.

Materials	k- point grid	g- point grid	λ	Materials	k- point grid	g- point grid	λ
(MoSSe) ₂ -Li	16×16×1	8×8×1	0.77	(WSSe) ₂ -Ca	16×16×1	8×8×1	1.44
	20×20×1	10×10×1	0.84		20×20×1	10×10×1	1.48
	24×24×1	12×12×1	0.84		24×24×1	12×12×1	1.48
(MoSSe) ₂ -Na	16×16×1	8×8×1	0.47	(WSSe) ₂ -K	16×16×1	8×8×1	1.64
	20×20×1	10×10×1	0.51		20×20×1	10×10×1	1.69
	24×24×1	12×12×1	0.51		24×24×1	12×12×1	1.69
(MoSSe) ₂ -Mg	16×16×1	8×8×1	0.53	(WSSe) ₂ -Sr	16×16×1	8×8×1	1.63
	20×20×1	10×10×1	0.56		20×20×1	10×10×1	1.68
	24×24×1	12×12×1	0.56		24×24×1	12×12×1	1.68
(MoSSe) ₂ -Ca	16×16×1	8×8×1	0.85	MoSSe-Li-WSSe	16×16×1	8×8×1	0.93
	20×20×1	10×10×1	0.92		20×20×1	10×10×1	0.98
	24×24×1	12×12×1	0.92		24×24×1	12×12×1	0.98
(MoSSe) ₂ -K	16×16×1	8×8×1	1.01	MoSSe-Na-WSSe	16×16×1	8×8×1	0.88
	20×20×1	10×10×1	1.05		20×20×1	10×10×1	0.91
	24×24×1	12×12×1	1.05		24×24×1	12×12×1	0.91
(MoSSe) ₂ -Sr	16×16×1	8×8×1	0.99	MoSSe-Mg-WSSe	16×16×1	8×8×1	0.55
	20×20×1	10×10×1	1.04		20×20×1	10×10×1	0.57
	24×24×1	12×12×1	1.04		24×24×1	12×12×1	0.57
(WSSe) ₂ -Li	16×16×1	8×8×1	0.69	MoSSe-Ca-WSSe	16×16×1	8×8×1	1.93
	20×20×1	10×10×1	0.74		20×20×1	10×10×1	1.98
	24×24×1	12×12×1	0.74		24×24×1	12×12×1	1.98
(WSSe) ₂ -Na	16×16×1	8×8×1	0.52	MoSSe-K-WSSe	16×16×1	8×8×1	2.07
	20×20×1	10×10×1	0.58		20×20×1	10×10×1	2.12
	24×24×1	12×12×1	0.58		24×24×1	12×12×1	2.12
(WSSe) ₂ -Mg	16×16×1	8×8×1	0.53	MoSSe-Sr-WSSe	16×16×1	8×8×1	1.71
	20×20×1	10×10×1	0.57		20×20×1	10×10×1	1.78
	24×24×1	12×12×1	0.57		24×24×1	12×12×1	1.78

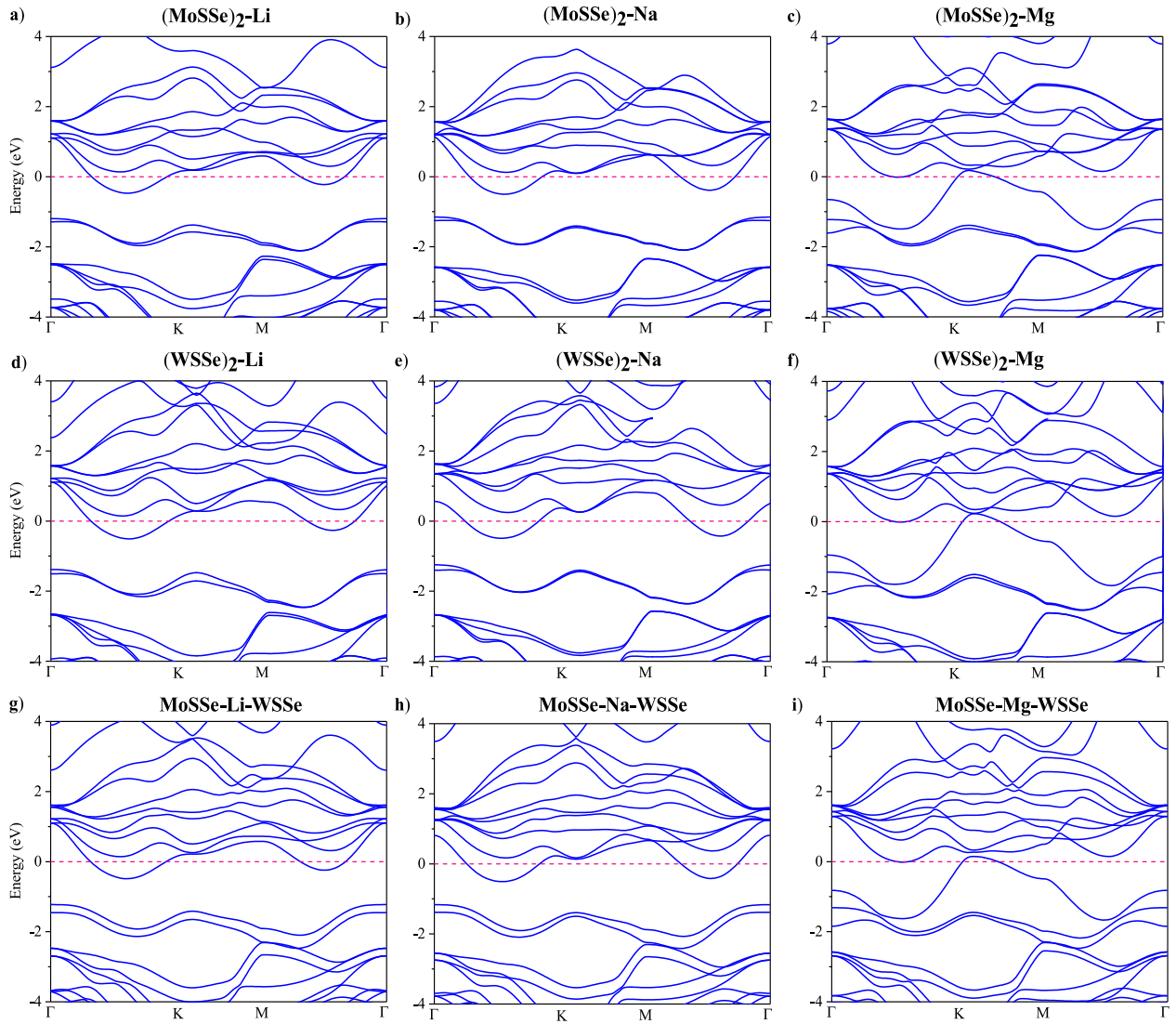


Fig. S1 Calculated electronic band structures of Janus MSSe ($M = \text{Mo}$ or W) bilayer and Janus MoSSe/WSSe heterostructure intercalated with the alkali metal (Li, Na) or alkaline earth metals (Mg).

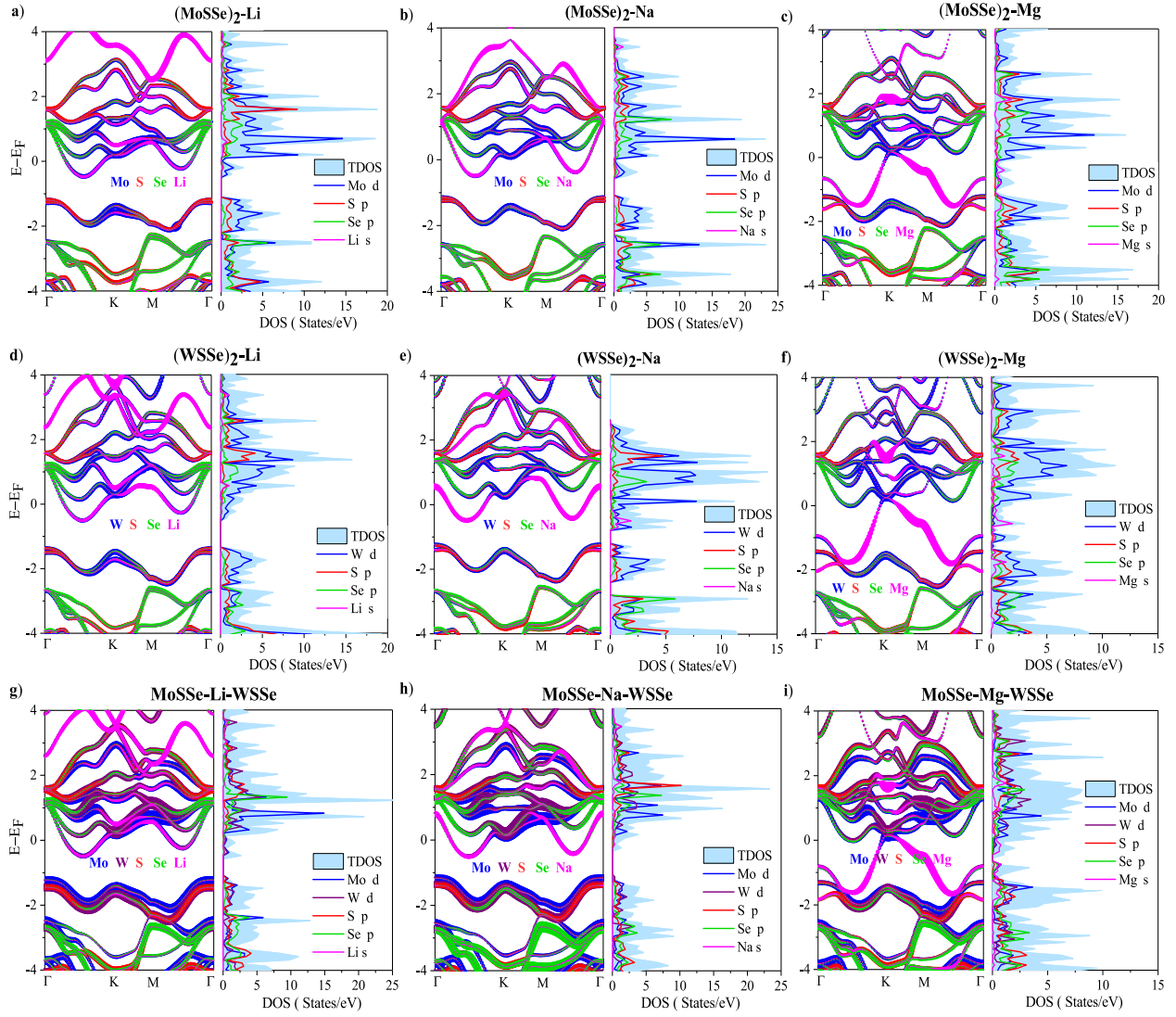


Fig. S2 The projected band structures, electronic total, and partial DOS calculated of Janus MSSe ($M = \text{Mo}$ or W) bilayer and Janus MoSSe/WSSe heterostructure intercalated with the alkali metal (Li, Na) or alkaline earth metals (Mg).

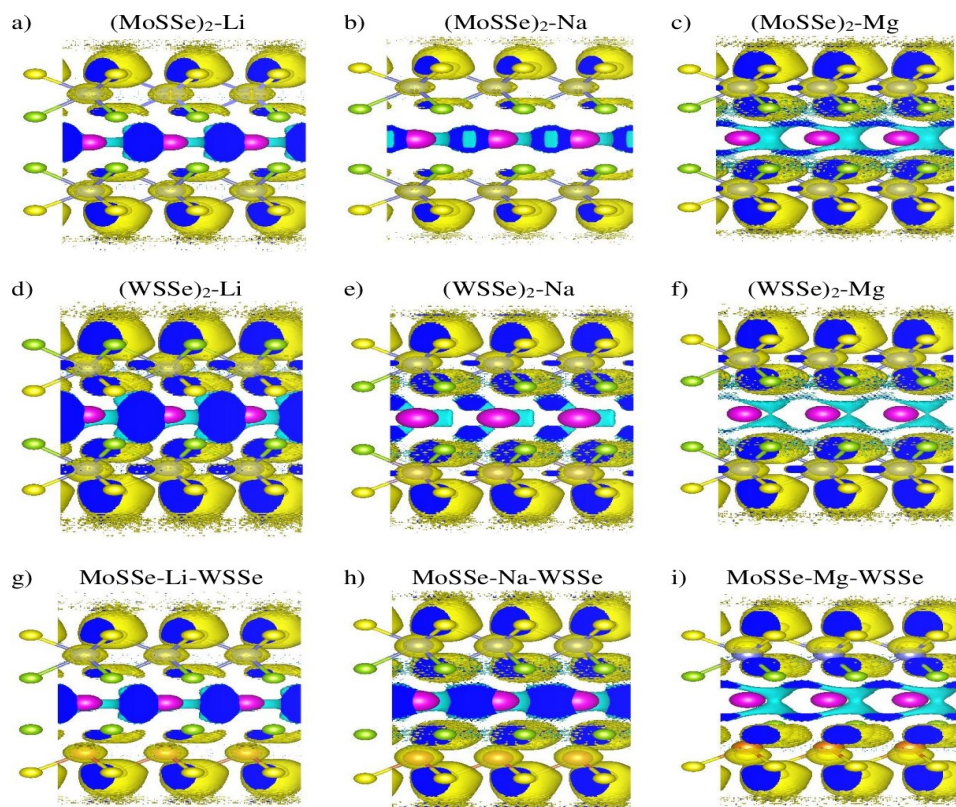


Fig. S3 The charge density difference plots for Janus MSSe ($M = \text{Mo}$ or W) bilayer and Janus MoSSe/WSSe heterostructure intercalated with the alkali metal (Li, Na) or alkaline earth metals (Mg).

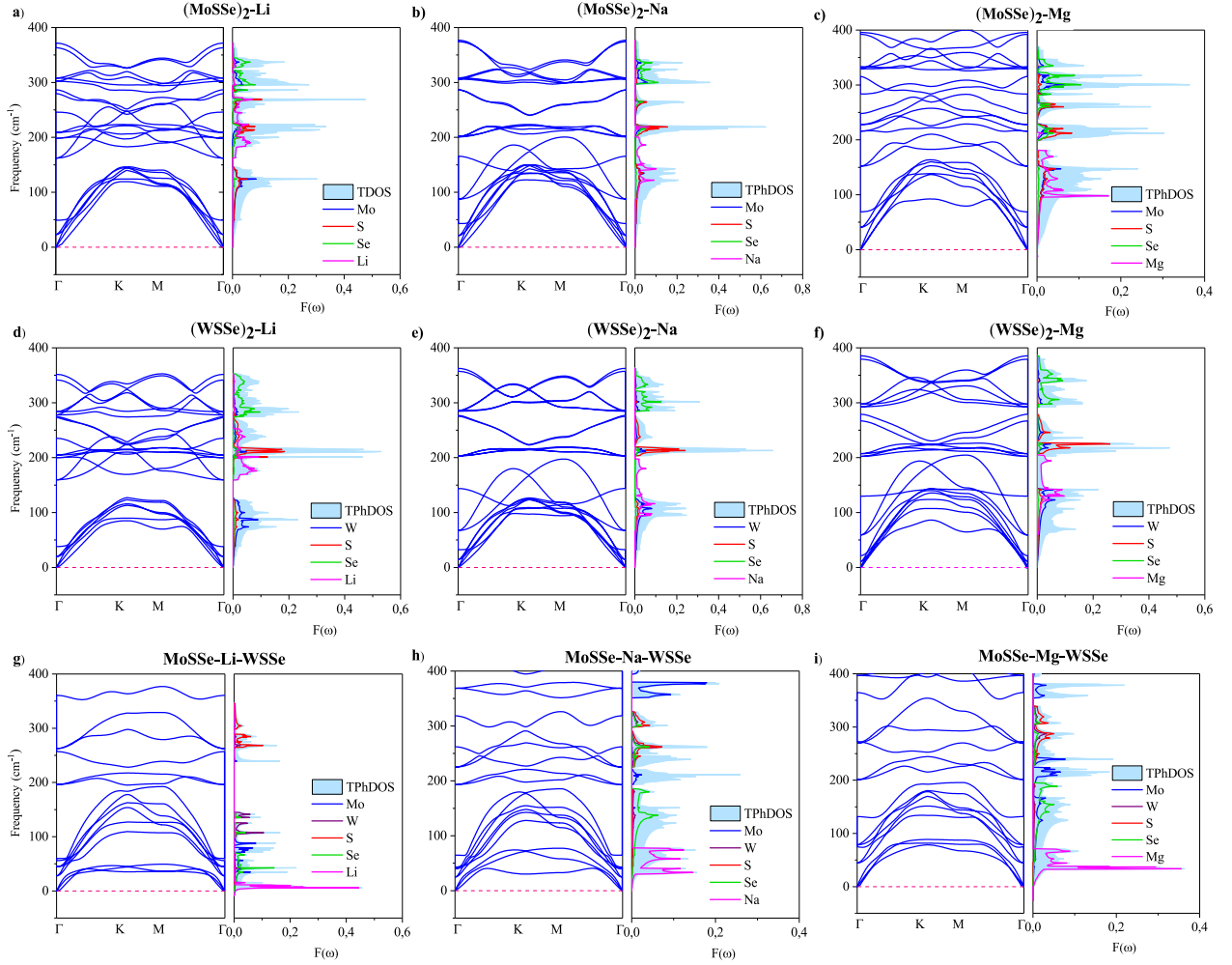


Fig. S4 The phonon dispersion and phonons density of states for Janus MSSe ($M = \text{Mo}$ or W) bilayer and Janus MoSSe/WSSe heterostructure intercalated with the alkali metal (Li, Na) or alkaline earth metals (Mg).

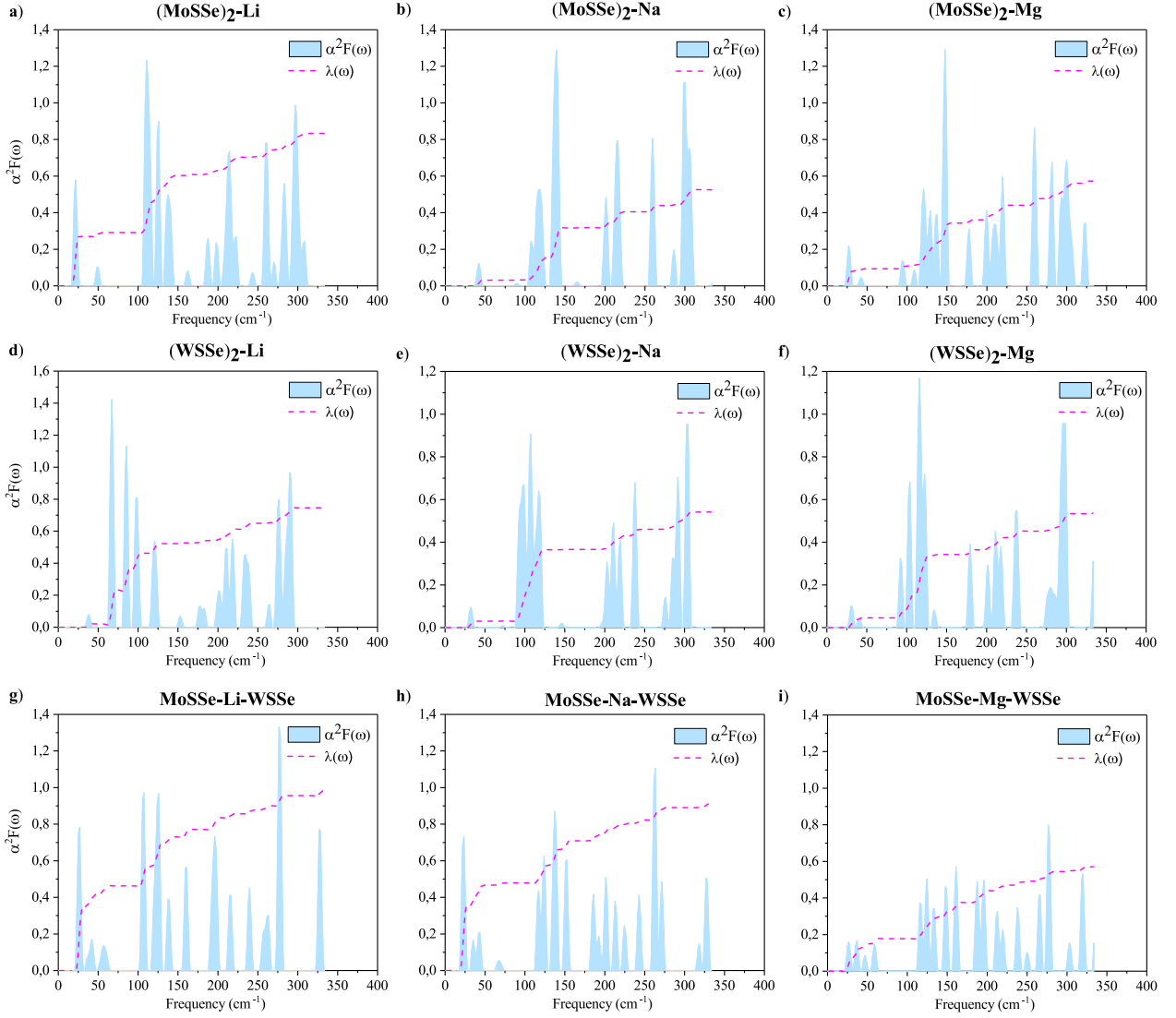


Fig. S5 Calculated spectral function for Janus MSSe ($M = \text{Mo}$ or W) bilayer and Janus MoSSe/WSSe heterostructure intercalated with the alkali metal (Li, Na) or alkaline earth metals (Mg).

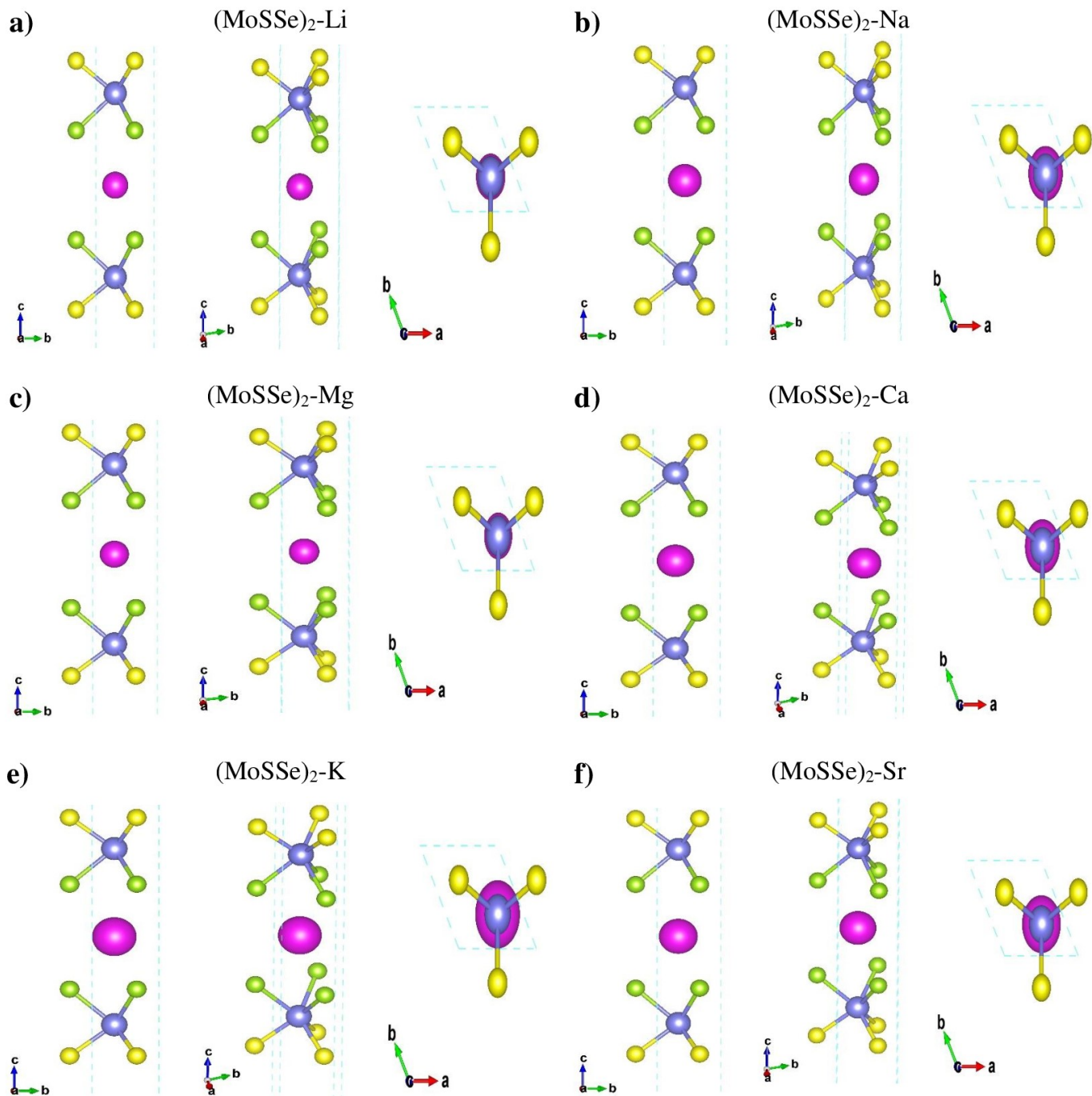


Fig. S6 The crystal structure of Janus MoSSe intercalated with the alkali metal (Li, Na, K) or alkaline earth metals (Mg, Ca, Sr).

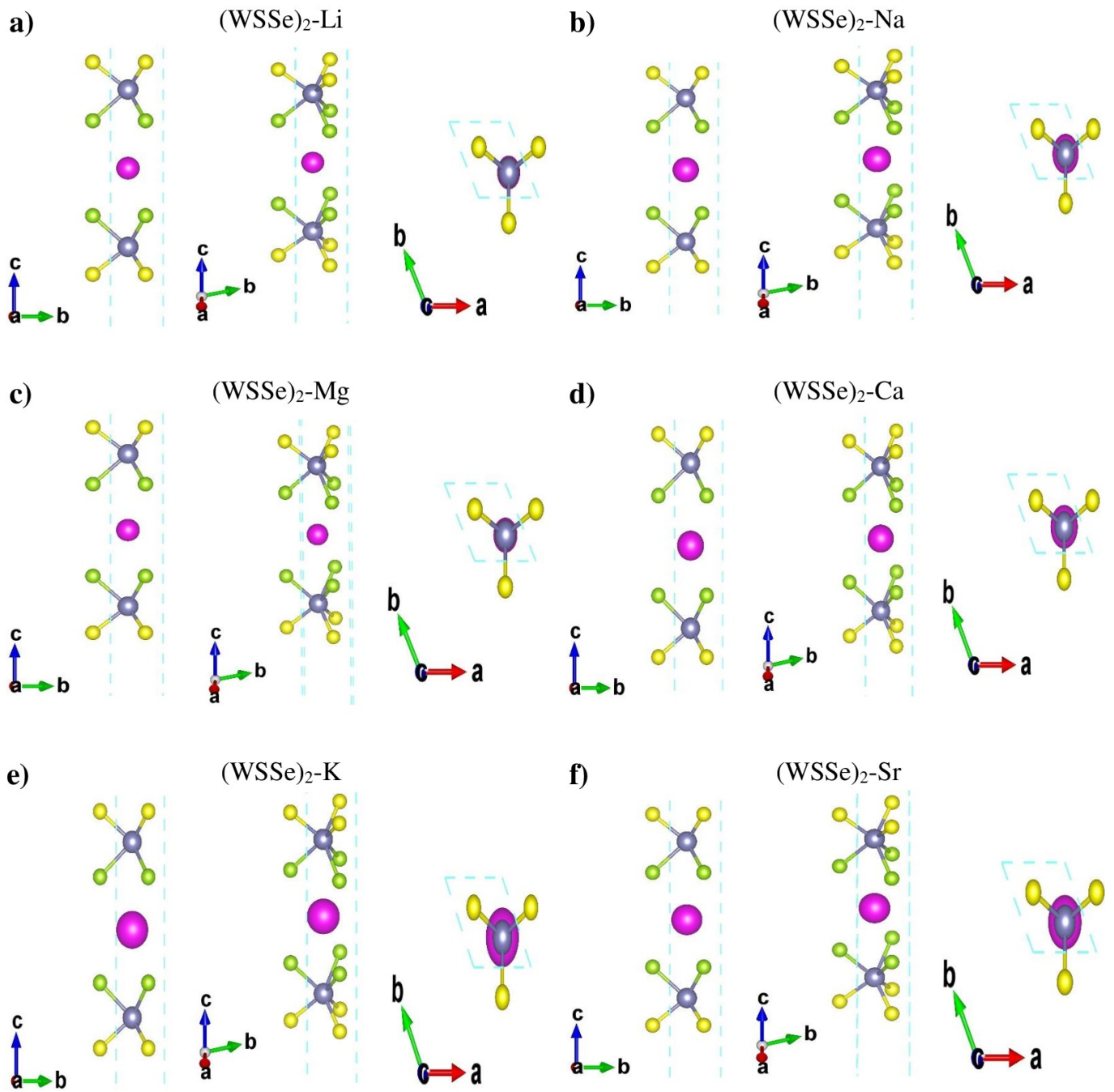


Fig. S7 The crystal structure of Janus WSSe intercalated with the alkali metal (Li, Na, K) or alkaline earth metals (Mg, Ca, Sr).

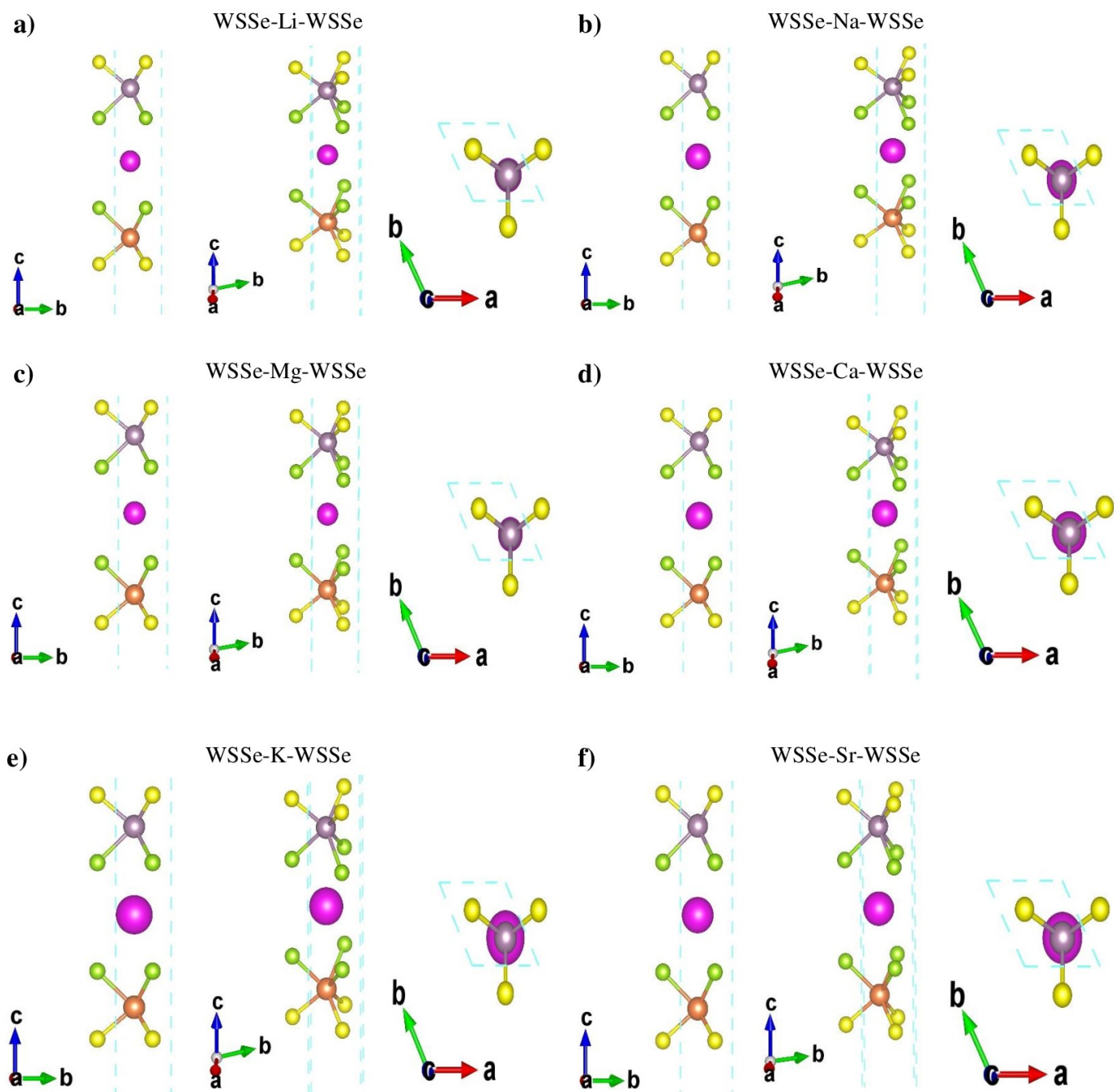


Fig. S8 The crystal structure of Janus MoSSe/WSSe heterostructure intercalated with the alkali metal (Li, Na, K) or alkaline earth metals (Mg, Ca, Sr).