Janus structures of SMoSe and SVSe compositions with low enthalpy and unusual crystal chemistry

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Table S1: Structural data SMoSe-O, O', and M".

Phase	Space group	Lattice parameters (Å, deg)			Atom	Coordinates		
						x	y	z
SMoSe-O	$Pmm2$ (#25)	$a = 5.6497$	$b = 3.2416$	$c = 23.0295$	Mo	0.2432	0.5	0.5028
		α = 90.000	β=90.000	γ=90.000	S	0.0000	0	0.5628
					S	0.5000	0.5	0.5815
					Se	0.0000	0	0.4342
					Se	0.5000	0.5	0.4159
SMoSe-O'	$Pmm2$ (#25)	$a = 11.8737$	$b = 3.1617$	$c = 26.1470$	Mo	0.1113	0.5	0.5006
		α = 90.000	β=90.000	γ=90.000	Mo	0.3330	0	0.5000
					S	0.0000	0	0.5563
					S	0.5000	0	0.5516
					S	0.2605	0.5	0.5618
					Se	0.0000	0	0.4385
					Se	0.5000	0	0.4377
					Se	0.2573	0.5	0.4319
SMoSe-M"	Pm (#6)	$a = 6.4527$	$b = 9.3860$	$c = 25.1952$	Mo	0.0177	0.7861	0.4954
		α = 90.000	β=90.179	γ=90.000	Mo	0.4825	0.7898	0.4967
					Mo	0.3301	0.5000	0.4961
					Mo	0.6747	0.5000	0.4970
					S	0.0102	0.0000	0.4509
					S	0.4903	0.0000	0.4433
					S	0.7476	0.6923	0.4359
					S	0.2535	0.6859	0.4320
					Se	0.0605	0.0000	0.5646
					Se	0.4419	0.0000	0.5639
					Se	0.7490	0.7008	0.5648
					Se	0.2508	0.6822	0.5673

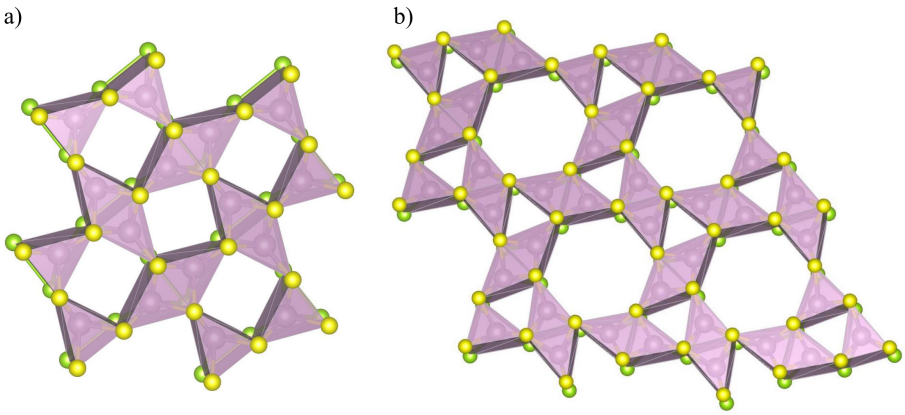

Figure S1: Packing of trigonal prisms in 1S (a) and 1H' (b) structures of SMoSe.

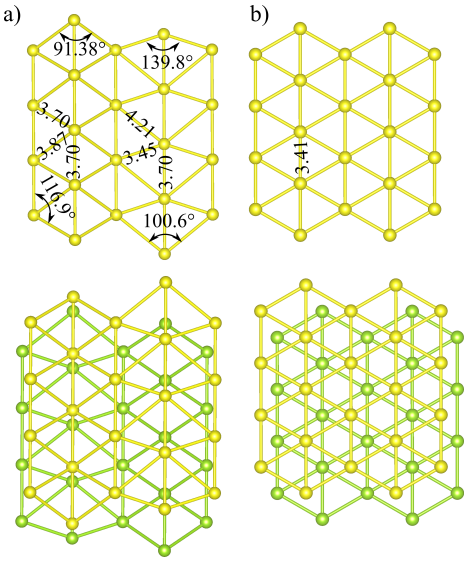

Figure S2: Comparison of the nets of Ch atoms in 1M (a) and 1T (b) crystal structures; sulphur is shown in yellow, selenium – in green.

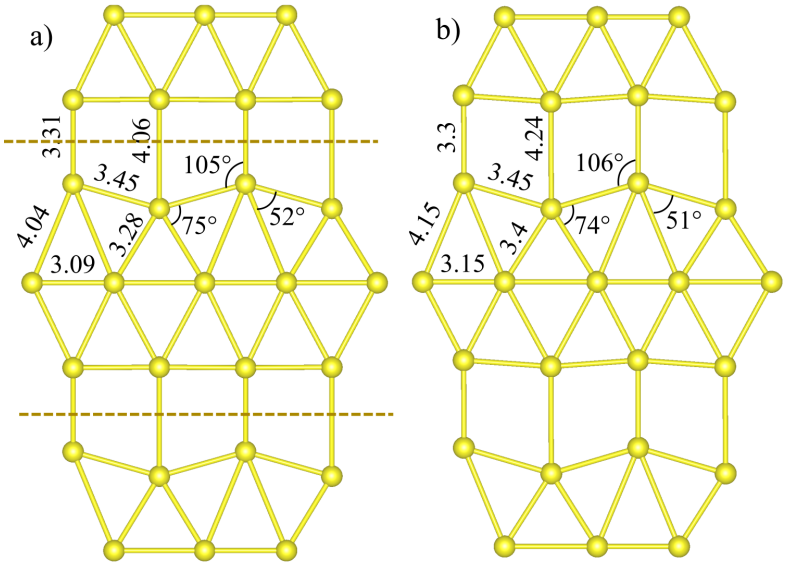

Figure S3: Interatomic distances and bond angles of sulphr nets in SVSe-1A (a) and SMoSe-1A' (b).

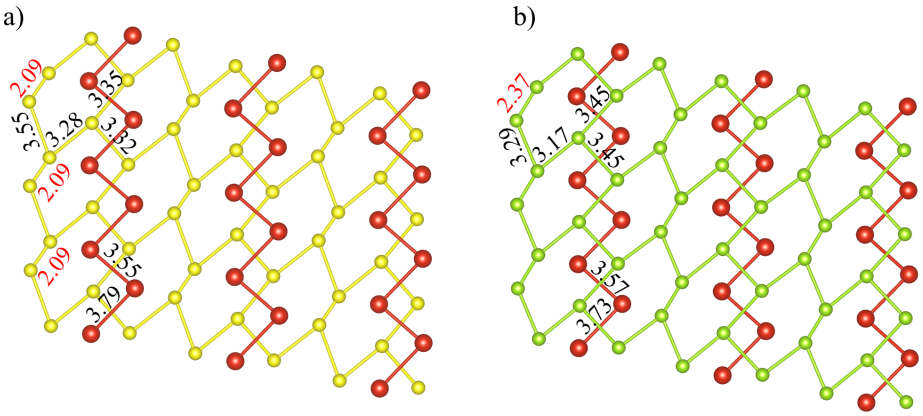

Figure S4: The net of sulphur (a) and selenium (b) atoms in SVSe-1A" crystal structure.