Supporting Information for the manuscript

Stabilities and Reconstructions of Clean PbS and PbSe Surfaces: DFT Results and the Role of Dispersion Forces

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Table S1 (*as supplement to Table 3 in the main text*): Surface Energies of Pristine and Reconstructed PbS and PbSe (111) Surfaces at the DFT-PBE Level of Theory

		γ (meV Å^{-2}), PBE			
		PbS		**PbSe**	
	term.	Pb poor[a]	Pb rich[b]	Pb poor[c]	Pb rich[b]
pristine	Pb	90	55	84	49
	S/Se	51	87	39	74
SV	Pb	45	27	43	26
	S/Se	38	55	32	49
MgO	Pb	72	54	69	51
	S/Se	67	85	57	74
2×1	Pb	22	22	20	20
	S/Se	27	27	26	26
oct	Pb	21	21	21	21
	S/Se	21	21	20	20

[a]Defined as $\mu_{\mathrm{Pb}} = E_{\mathrm{PbS}}^{(\mathrm{bulk})} - E_{\mathrm{S}}^{(\mathrm{bulk})}$. [b]In both cases, defined as $\mu_{\mathrm{Pb}} = E_{\mathrm{Pb}}^{(\mathrm{bulk})}$. [c]Here, $\mu_{\mathrm{Pb}} = E_{\mathrm{PbSe}}^{(\mathrm{bulk})} - E_{\mathrm{Se}}^{(\mathrm{bulk})}$.

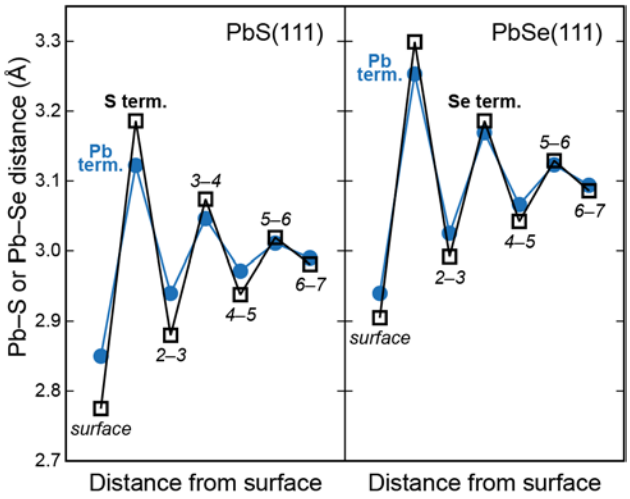

Figure S2 (*as supplement to Figure 3 in the main text*): Course of Pb–S and Pb–Se bond lengths near the relaxed, pristine (111) surfaces. Results at the PBE level of theory are shown.

Table S2 (*as supplement to Table 4 in the main text*): Structural Properties of Reconstructed PbS and PbSe (111) Surfaces at the PBE Level of Theory[a]

			d_1 (Å)	d_2 (Å)	d_3 (Å)
PbS	(2×1)	Pb-term.	2.65	2.77	—
		S-term.	2.63	2.78	—
	oct.	Pb-term.	2.72	2.82	2.85
		S-term.	2.73	2.77	2.95
PbSe	(2×1)	Pb-term.	2.78	2.89	—
		Se-term.	2.78	2.91	—
	oct.	Pb-term.	2.84	2.95	2.96
		Se-term.	2.86	2.89	3.07

[a]The parameters d_1, d_2, and d_3 are defined in Figure 4 in the main text.