Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
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Supporting Information:

Table 1 Optimized cell parameters (a, c) and calculated total energies (E_{tot}) of 2H and 3R polytypes of MoS_2 cell, and d_{Mo-S} is bond length.

Phase	Method	a (Å)	c (Å)	d_{Mo-S} (Å)	E_{tot} (eV/MoS_2)
	PBE	3.18	14.74	2.41	-21.80
2H-MoS_2	DFT-D2	3.19	12.36	2.41	-22.55
	vdW-DF	3.22	12.67	2.44	-20.20
	PBE	3.19	21.17	2.41	-21.80
3R-MoS_2	DFT-D2	3.19	18.55	2.41	-22.55
	vdW-DF	3.22	18.96	2.44	-20.20

The optimized lattice constants and atomic structural parameters of these MoS_2 polytypes are presented in Table 1. Our results are in good agreement with previous theoretical results. Using the same vdW-DF method, Rydberg *et al*[31] reported a = 3.3 Å, and c = 12.6 Å for 2H-MoS_2, which are qualitatively similar to our results (a = 3.22 Å, and c = 12.67 Å). Mortazavi *et al*[32] obtained a = 3.19 Å, and c = 18.52 Å for 3R phase with the DFT-D2 method.