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

Supplementary Information

Chirality dependent electromechanical properties of single-layer MoS_2 under out-of-plane deformation: A DFT study

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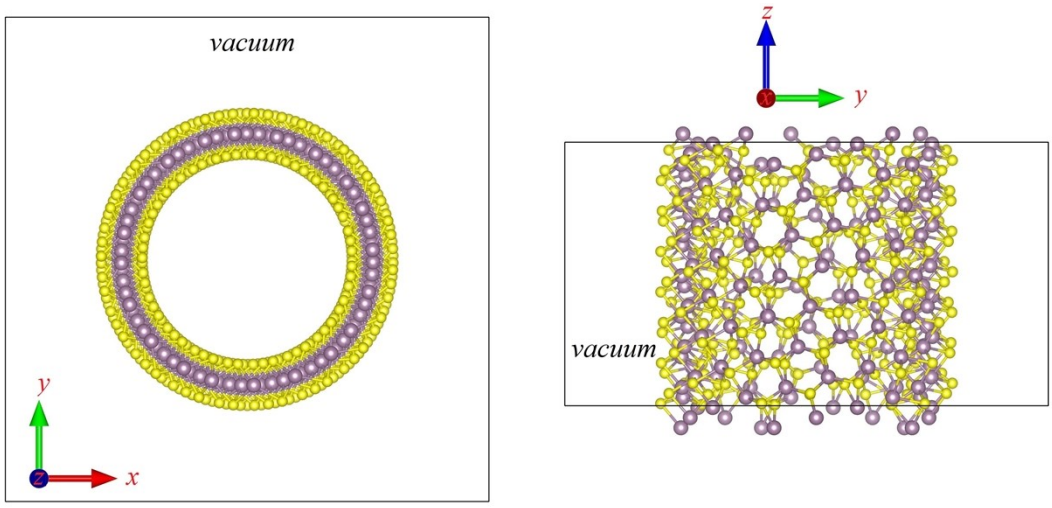

Figure S1. Top (left) and side (right) views of schematic of a MoS_2 nanotube.

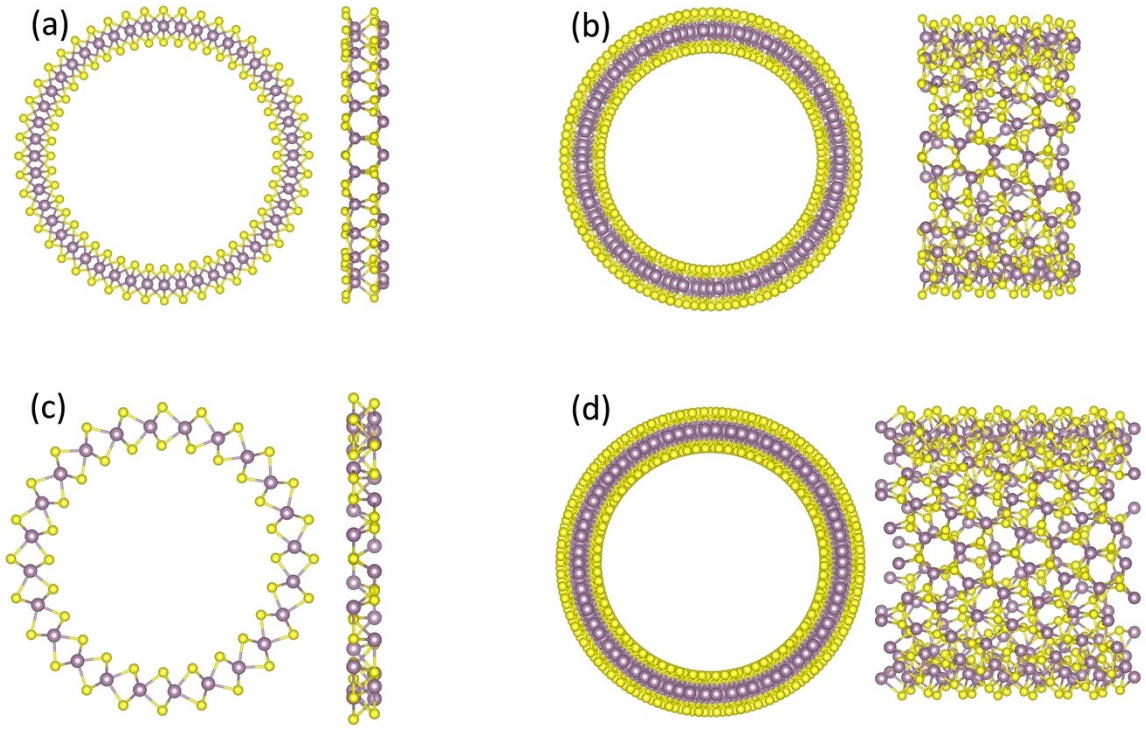

Figure S2. Top (left) and side (right) views of unit cells for (a) (1, 1), (b) (2, 1), (c) (3, 1) and (d) (4, 1) MoS_2 nanotube with a diameter of ~21 Å.

Table 1. Number of atoms (N_{atom}) and S-Mo bond lengths (Å) of MoS_2 nanotube models rolling along different in-plane directions as a dependence of diameters (Å).

Tube-type	Diameter	N_{atom}	S1-Mo	S2-Mo	S3-Mo	S4-Mo	S5-Mo	S6-Mo
(1, 1)	**9.70**	48	2.39	3.55	2.49	2.40	2.36	2.36
	13.38	72	2.53	2.53	2.40	2.38	2.38	2.34
	17.10	98	2.49	2.49	2.41	2.38	2.38	2.36
	20.96	120	2.47	2.47	2.41	2.38	2.38	2.37
	24.84	144	2.46	2.46	2.41	2.38	2.38	2.38
	32.76	192	2.44	2.44	2.41	2.39	2.39	2.39
(2, 1)	**8.35**	24	2.38	2.38	2.30	2.37	2.37	4.43
	11.55	36	2.45	2.45	2.61	2.36	2.36	2.37
	14.79	48	2.44	2.44	2.54	2.37	2.37	2.37
	21.48	72	2.43	2.43	2.48	2.38	2.38	2.37
	28.34	96	2.43	2.43	2.46	2.39	2.39	2.38
	31.84	108	2.42	2.42	2.45	2.39	2.39	2.38
	37.05	126	2.42	2.42	2.46	2.39	2.39	2.38
(3, 1)	**9.51**	126	2.42	2.49	2.74	2.33	2.36	2.40
	11.84	168	2.43	2.47	2.61	2.35	2.37	2.38
	14.31	210	2.42	2.46	2.55	2.36	2.37	2.38
	16.83	252	2.42	2.45	2.52	2.37	2.38	2.37
	21.97	336	2.42	2.44	2.48	2.38	2.38	2.38
	27.17	420	2.42	2.43	2.46	2.39	2.39	2.38
	35.01	546	2.42	2.44	2.46	2.39	2.39	2.38
(4, 1)	**8.99**	156	2.39	2.52	2.82	2.32	2.37	2.41
	12.16	234	2.48	2.51	2.60	2.40	2.40	2.39
	15.53	312	2.42	2.47	2.53	2.36	2.38	2.38
	18.92	390	2.42	2.46	2.49	2.37	2.38	2.38
	22.45	468	2.42	2.45	2.48	2.38	2.38	2.38
	26.00	546	2.42	2.44	2.46	2.39	2.38	2.38
	29.59	624	2.42	2.44	2.46	2.39	2.39	2.38