

Table S1. Energetic and structural properties of double-walled (DW NT) and merged single-walled (CSW NT) TiO₂ NTs obtained from layers with hexagonal fluorite morphology. Comparison of results obtained using PBE0 and PBE0-D methods.

Nanotube, armchair		E_f^a		E_{str}^a		E_{bind}^a		w_{NT}^b		D_{NT}^c	
		kJ/mol				Å					
		PBE0	PBE0-D	PBE0	PBE0-D	PBE0	PBE0-D	PBE0	PBE0-D	PBE0	PBE0-D
(12, 12)@(18, 18)	DW NT	47.5	72.9	3.9	-4.2	-3.5	-13.4	2.0	2.0	24.7	24.6
	CSW NT	48.5	76.0	4.9	-1.1	-2.5	-10.3	5.9	5.9	25.3	25.3
(10, 10)@(15, 15)	DW NT	53.1	77.8	9.5	0.7	-1.1	-12.9	1.9	1.9	20.7	20.7
	CSW NT	44.5	71.2	0.9	-5.9	-9.7	-19.4	5.4	4.9	22.1	21.8

^aFormation energy, E_f , strain energy, E_{str} , and binding energy, E_{bind} .

^bThe average wall thickness in NT relaxed structures.

^cThe average diameter calculated as the sum of radial distances to outmost and innermost (oxygen) atoms in NT relaxed structures.