

Supporting information

Structural and Electronic Properties of Double Wall MoSTe Nanotubes

Zhenyun Lan,^{*,a,b} Theresa Isabelle Manguerra Kapunan,^a Tejs Vegge,^a and Ivano E. Castelli^{*,a}

^aDepartment of Energy Conversion and Storage, Technical University of Denmark, Anker Engelundsvej 411, DK-2800 Kgs. Lyngby, Denmark. *E-mail:* zhenlan@dtu.dk; ivca@dtu.dk

^b School of Materials Science and Engineering, Hefei University of Technology, Hefei, Anhui 230009, PR China.

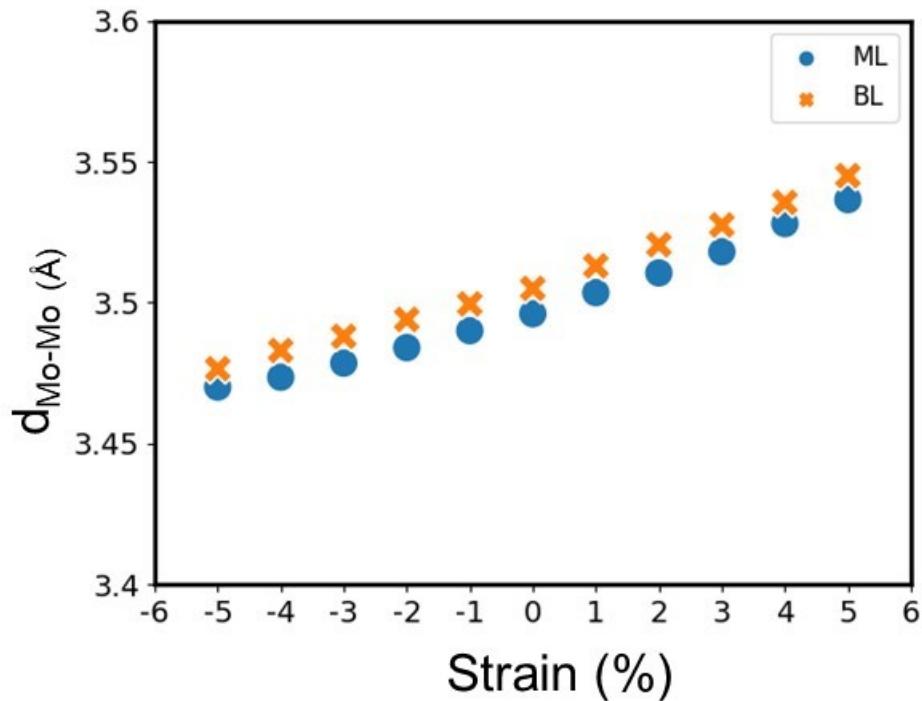


Figure S1. (a) The relationship between the Mo-Mo bond length for MLs, BLs, in blue, orange respectively and applied strain.

Table S1. The calculated band gap of 2D structures using HSE.

	Indirect band gap (eV)	Direct band gap (eV)
ML (Monolayer)	1.08	1.52
BL (Bilayer)	Metallic	0.45