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# Ultra-Stable Small Diameter Hybrid Transition Metal Dichalcogenide Nanotubes
## *X*-TM-*Y* (X, Y = S, Se, Te; TM = Mo, W, Nb, Ta)

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### The classical model

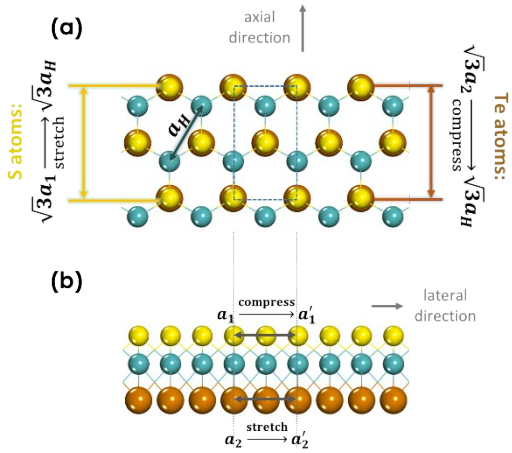


Fig. SI (a) When a flat SMoTe monolayer is rolled into a ZZ tube, we suppose its axial direction (also armchair direction, AC) lattice constant is fastened with $\sqrt{3}a_H$, which indicates the S-S distance along the axial direction is also $\sqrt{3}a_H$, i.e., **stretched** by ($\sqrt{3}a_H$ - $\sqrt{3}a_1$)/$\sqrt{3}a_1$ compared to that in pure $MoS_2$ tube, while the Te-Te distance is **compressed** by ($\sqrt{3}a_2$ - $\sqrt{3}a_H$)/$\sqrt{3}a_2$. (b) Then the S-S and Te-Te distance in the lateral direction will have opposite changes due to Poisson's effect, which makes $a_1$ shorten to $a'_1$ and $a_2$ lengthen to $a'_2$.

### Parameters and results

TABLE SI: The strip-tube transition diameter ($D_{s-t}$), optimal radii of *X*-TM-*Y* hybrid NTs obtained from the model ($R_O$) and from fitting to the DFT results ($R_{DFT}$) in the unit of nm, and the energy difference between a hybrid tube and the corresponding monolayer ($\varepsilon_{c0}$ in meV). The fitted coefficients $\alpha$ (eVÅ$^2$/atom) in Eq. (3), the in-plane lattice constants of the hybrid monolayer $a_H$ used in the model (the values in parenthesis are from DFT) and parameters found from literatures [1-4] are also listed. The Poisson's ratio of $TaTe_2$ is not available so it is set to 0.35, equal to $TaS_2$ and $TaSe_2$.

| X | TM | Y | $a_H$ | $v_1$ | $h_1$ | $a_1$ | $v_2$ | $h_2$ | $a_2$ | $R_O$ | $R_{DFT}$ | $D_{s-t}$ | $\varepsilon_{c0}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| S | Mo | Te | 3.38 (3.36) | 0.25 | 3.13 | 3.19 | 0.24 | 3.62 | 3.56 | 2.5 | 1.9 | 2.0 | -43 |
| Se | Mo | Te | 3.45 (3.42) | 0.23 | 3.35 | 3.33 | 0.24 | 3.62 | 3.56 | 4.2 | 3.0 | 3.0 | -20 |
| S | Mo | Se | 3.26 (3.26) | 0.25 | 3.13 | 3.19 | 0.23 | 3.35 | 3.33 | 6.1 | 4.2 | 3.1 | -8 |
| S | W | Te | 3.38 (3.36) | 0.22 | 3.14 | 3.19 | 0.18 | 3.63 | 3.56 | 2.6 | 1.9 | 2.2 | -48 |
| Se | W | Te | 3.44 (3.42) | 0.19 | 3.36 | 3.32 | 0.18 | 3.63 | 3.56 | 4.2 | 3.2 | 3.2 | -19 |
| S | W | Se | 3.26 (3.26) | 0.22 | 3.14 | 3.19 | 0.19 | 3.36 | 3.32 | 6.7 | 4.2 | 3.2 | -9 |
| S | Nb | Te | 3.53 (3.53) | 0.38 | 3.14 | 3.36 | 0.35 | 3.69 | 3.70 | 2.6 | 2.3 | 2.3 | -21 |
| Se | Nb | Te | 3.59 (3.60) | 0.36 | 3.37 | 3.48 | 0.35 | 3.69 | 3.70 | 4.3 | 3.8 | 3.6 | -8 |
| S | Nb | Se | 3.42 (3.43) | 0.38 | 3.14 | 3.36 | 0.36 | 3.37 | 3.48 | 6.7 | 5.1 | 4.1 | -4 |
| S | Ta | Te | 3.53 (3.52) | 0.35 | 3.13 | 3.34 | 0.35 | 3.66 | 3.71 | 2.4 | 2.0 | 2.3 | -33 |
| Se | Ta | Te | 3.60 (3.59) | 0.35 | 3.36 | 3.48 | 0.35 | 3.66 | 3.71 | 4.1 | 3.4 | 3.5 | -12 |
| S | Ta | Se | 3.41 (3.40) | 0.35 | 3.13 | 3.34 | 0.35 | 3.36 | 3.48 | 5.9 | 4.7 | 4.4 | -5 |

## Notes and references

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