Supplementary data for

Nanoleite: A new semiconducting carbon allotrope predicted by density functional theory

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1. The first three initial structure combination of lonsdaleite and (3,3), (6,6) and (9,9) carbon nanotubes, from left to right.

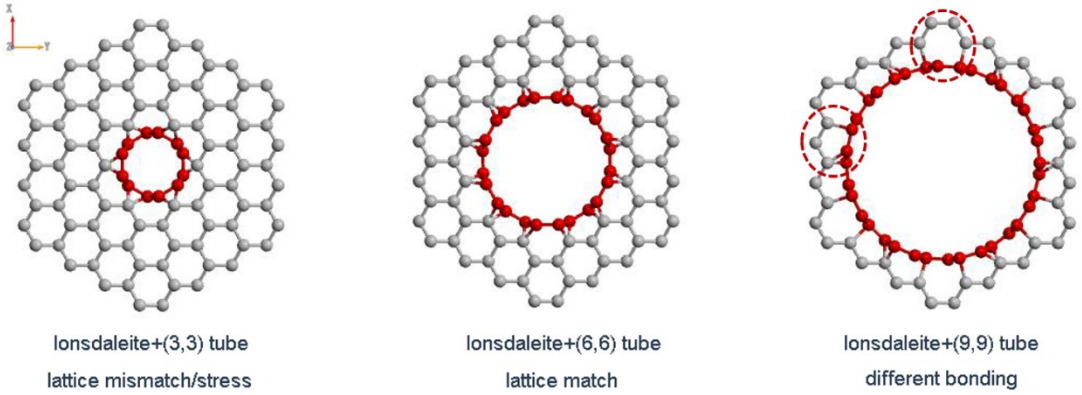

Fig. S1. Initial structure combination of lonsdaleite and (3,3), (6,6) and (9,9) carbon nanotubes, from left to right.

Fig. S1 shows the first three initial structure combination of lonsdaleite and (3,3), (6,6) and (9,9) carbon nanotubes. For the (3,3) tube, there exists a lattice mismatch because the hole formed in lonsdaleite is small compare to the diameter of the (3,3) tube. Thus large internal stress should be expected. In comparison, for the (6,6) tube, the lattice match is fulfilled and the carbon nanotube shows a uniform bonding environment. However, for the (9,9) tube, there exists different bonding environment, which may result in internal stress should also be expected. For even larger diameter tubes, such as (12, 12) or (15,15) tubes, which require much larger holes to accommodate the large diameter of tubes, leading to crystal structure with low mechanical properties thus is not an interesting focus for our current report.

2. The 3×3×1 supercell of nanoleite

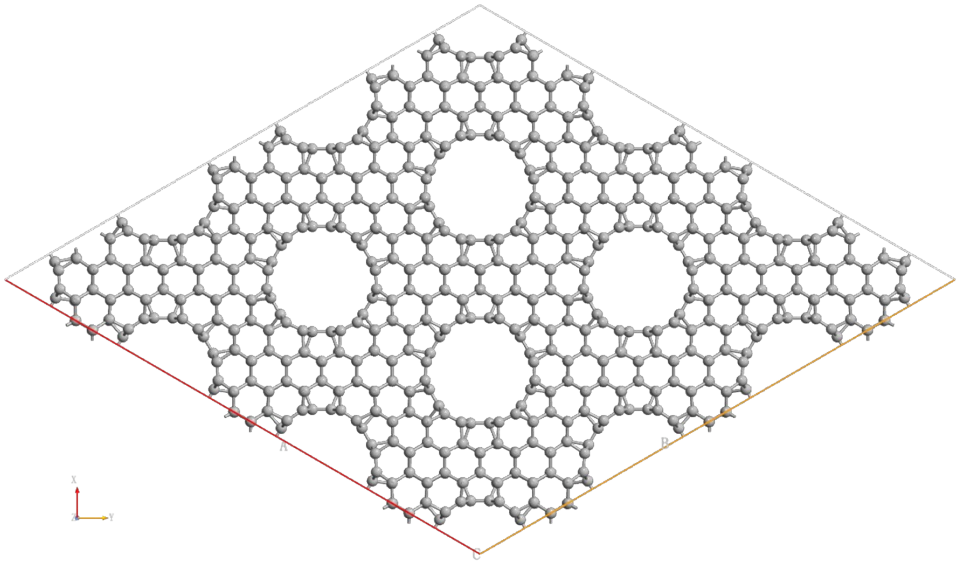

Fig. S2. The ball-stick 3×3×1 supercell of nanoleite

3. Snapshot of a free CNT (6,6) and its configuration after fully relaxed

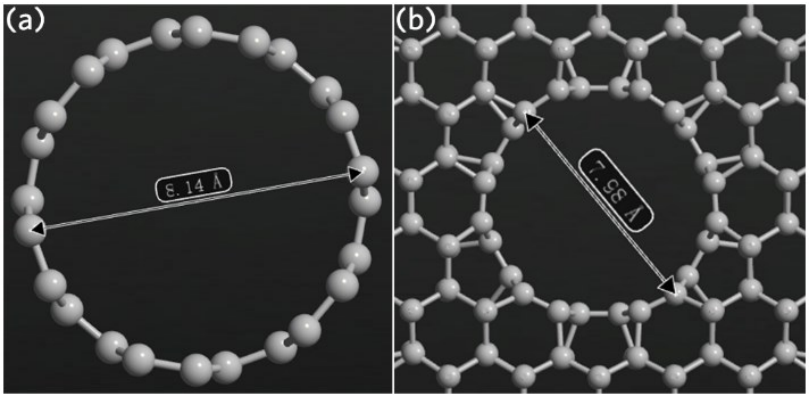

Fig. S3. (a) A free CNT (6,6), (b) within the lonsdaleite cavity after fully relaxed.