One-Dimensional Moiré Superlattices and Magic Angle Physics in Collapsed Chiral Carbon Nanotubes

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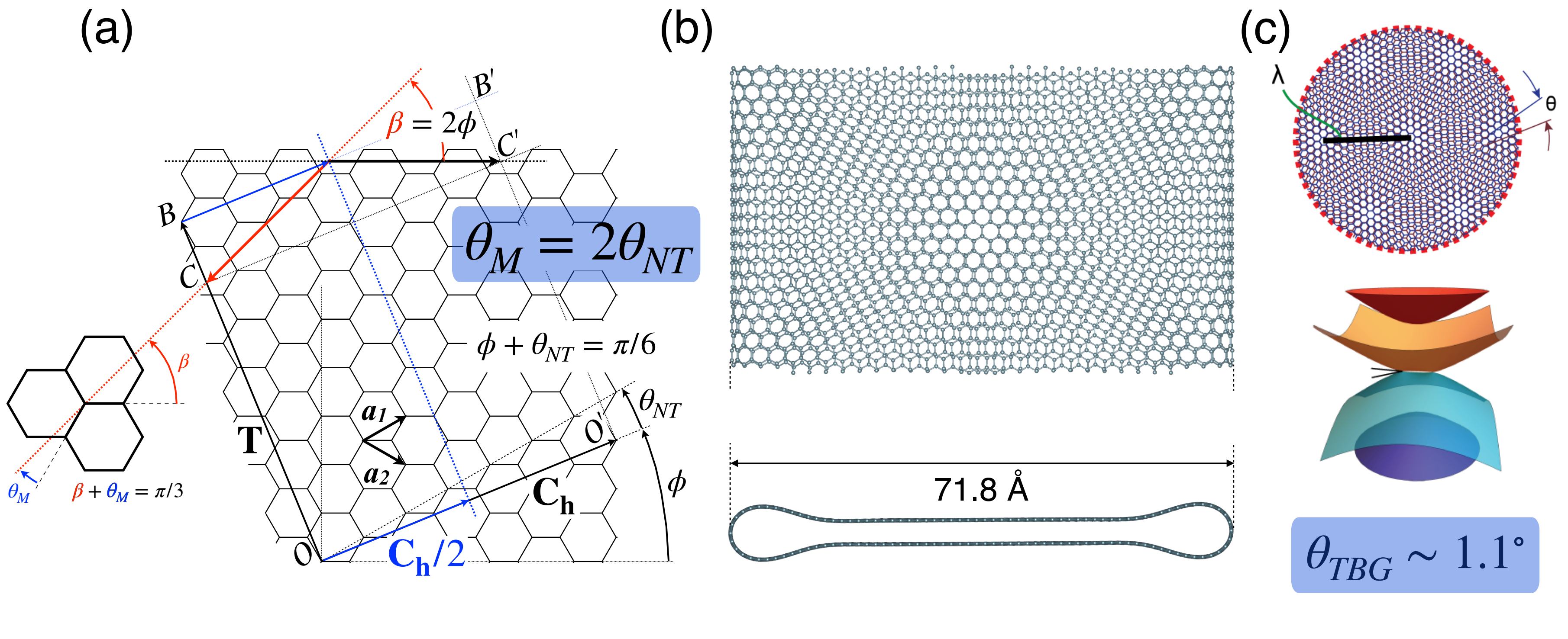
We demonstrate that one-dimensional moiré patterns, analogous to those found in well-known **twisted bilayer graphene** (TBG), can arise in collapsed **chiral carbon nanotubes** (CNTs). Resorting to a combination of approaches, namely, molecular dynamics to obtain the relaxed geometries and tight-binding calculations validated against *ab initio* modeling, we find that magic angle physics occur in collapsed carbon nanotubes. Chiral collapsed carbon nanotubes stand out as promising candidates to explore many-body effects, topology and superconductivity in low dimensions, emerging as the one-dimensional analogues of twisted bilayer graphene.

System geometry and motivation

Nanotubes are described by a chiral angle θ_{NT} and indices (n,m). For small θ_{NT}, moiré patterns can appear in CNTs. We find that the number and position of the moirés depend on the symmetry operations of the tube [1].

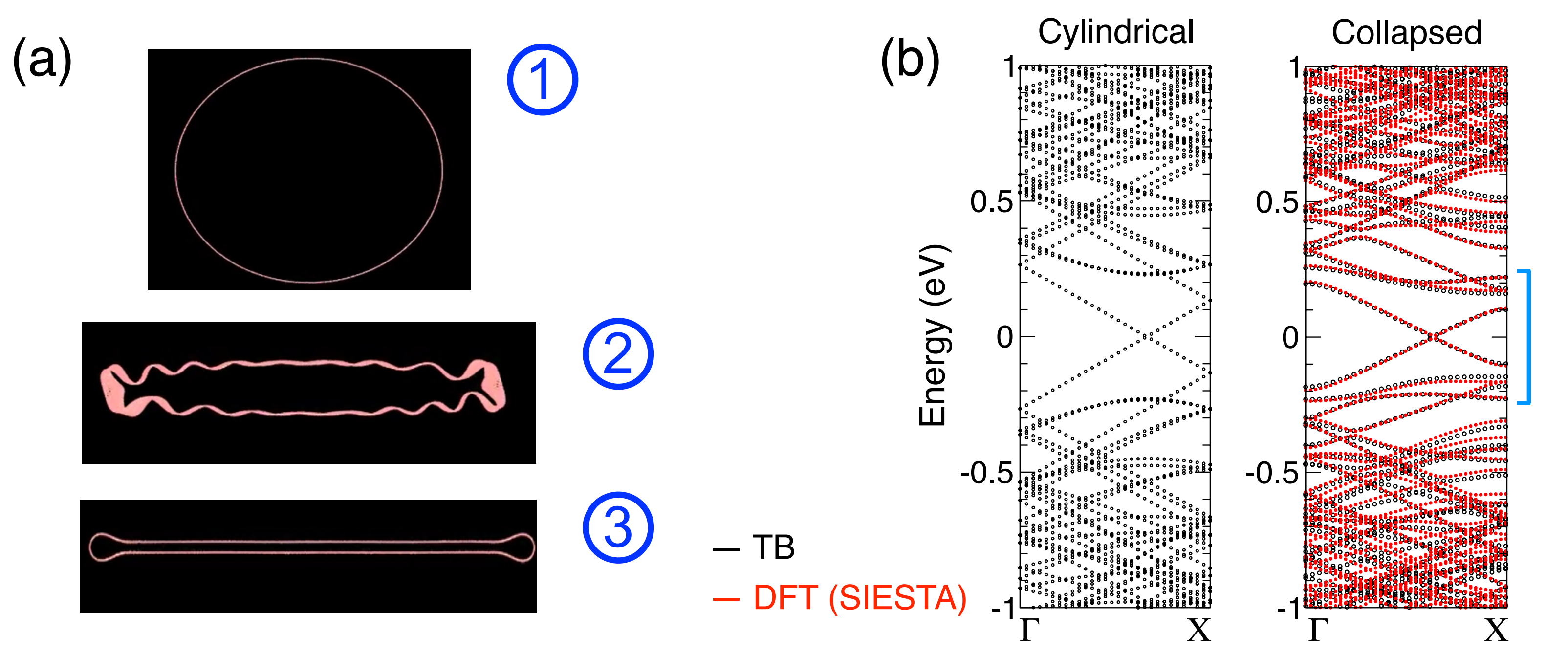


(a) Relation between the moiré and the chiral angle of a CNT. (b) Top view and cross section of a collapsed metallic CNT. (c) Moiré patterns and band velocity reduction in TBG [2].

Computational approach and methods

Tight-binding Hamiltonian [3]: $H = -\sum_{ij} t(R_i - R_j)\,|R_i\rangle\langle R_j| + H.c.$

Model validated against DFT simulations for the (62,2) (2648 atoms) and (36,2) (2744 atoms) CNTs.



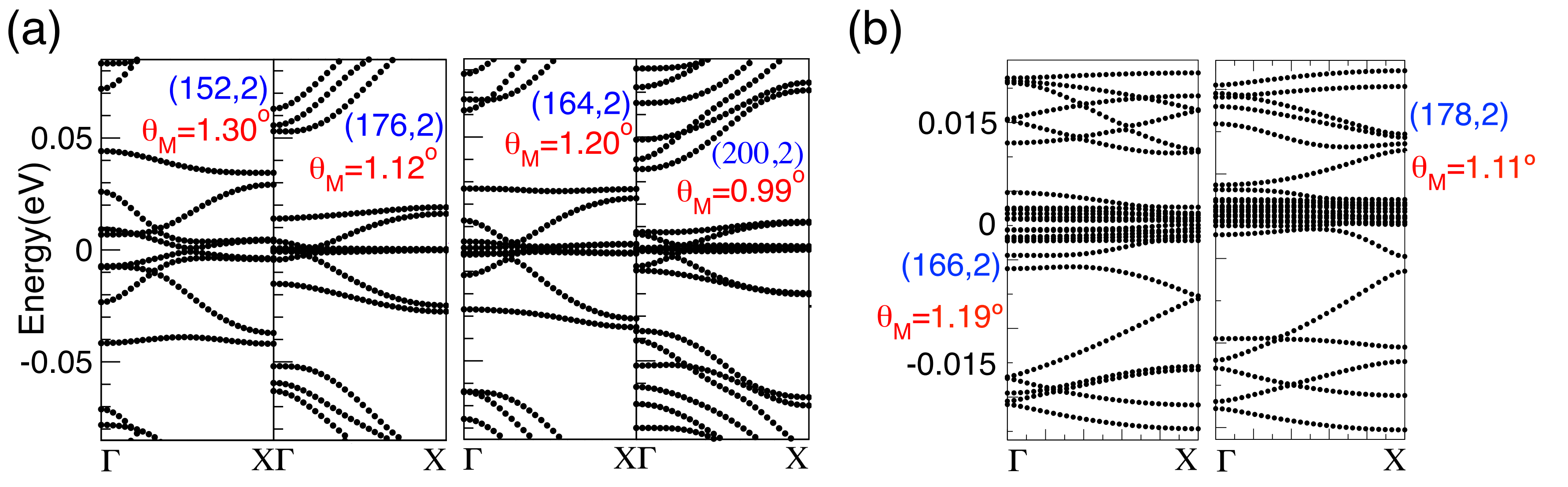
(a) Steps of the molecular dynamics relaxation process. (b) Band structures of the (62,2) CNT.

Evidences of magic angle physics

1. Flat bands and minimum bandwidth

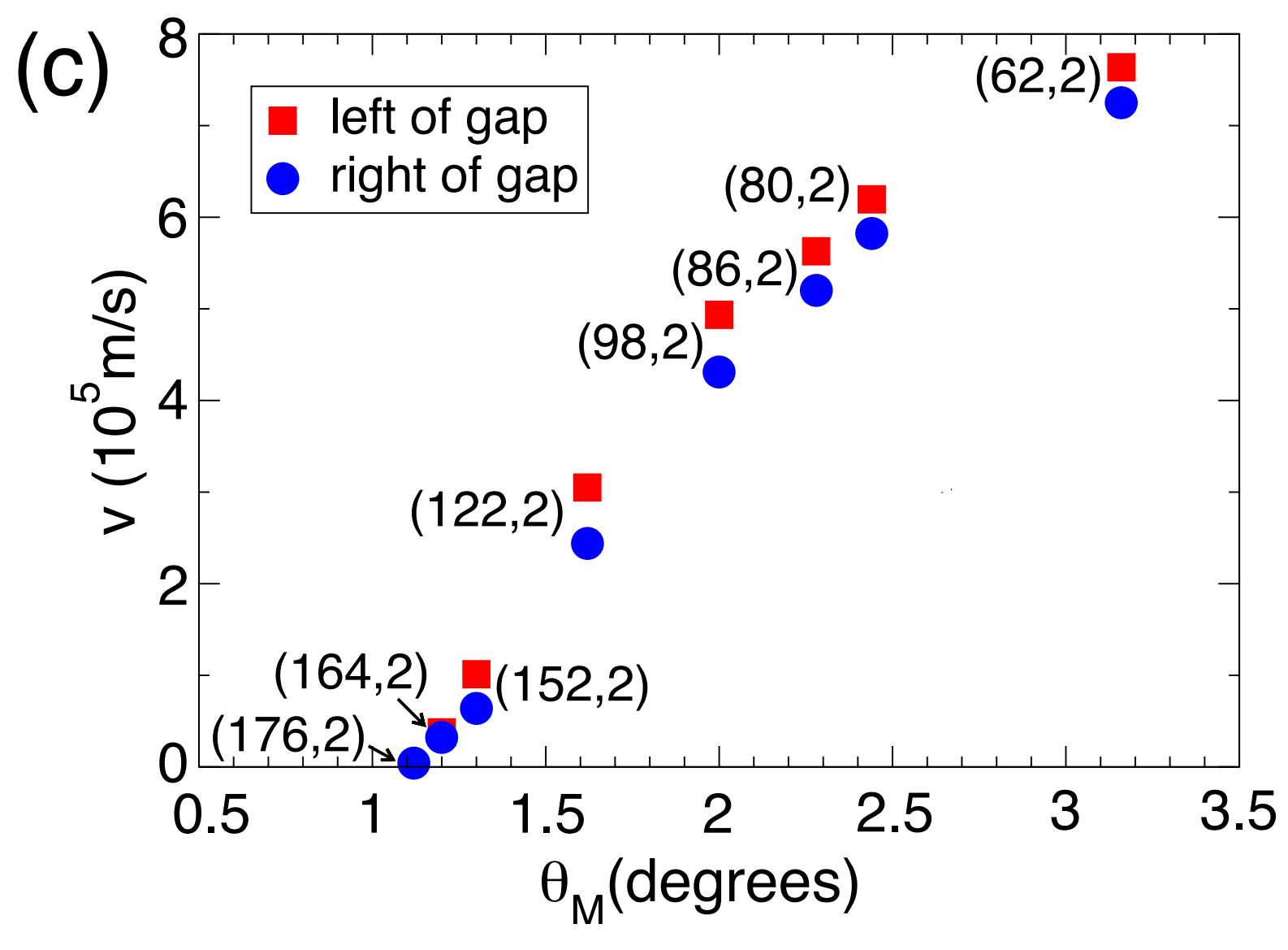
Metallic CNTs: 1 moiré/unit cell
- Central 8-band set
- 2 central flattest bands

Semiconducting CNTs: 3 moirés/u.c.
- Central 24-band set
- 10 central flattest bands [4]



Band structures of collapsed (a) metallic and (b) semiconducting CNTs. (c) Velocities of the conduction band near the gap for some tubes.

2. Velocity $v_F \sim 0$

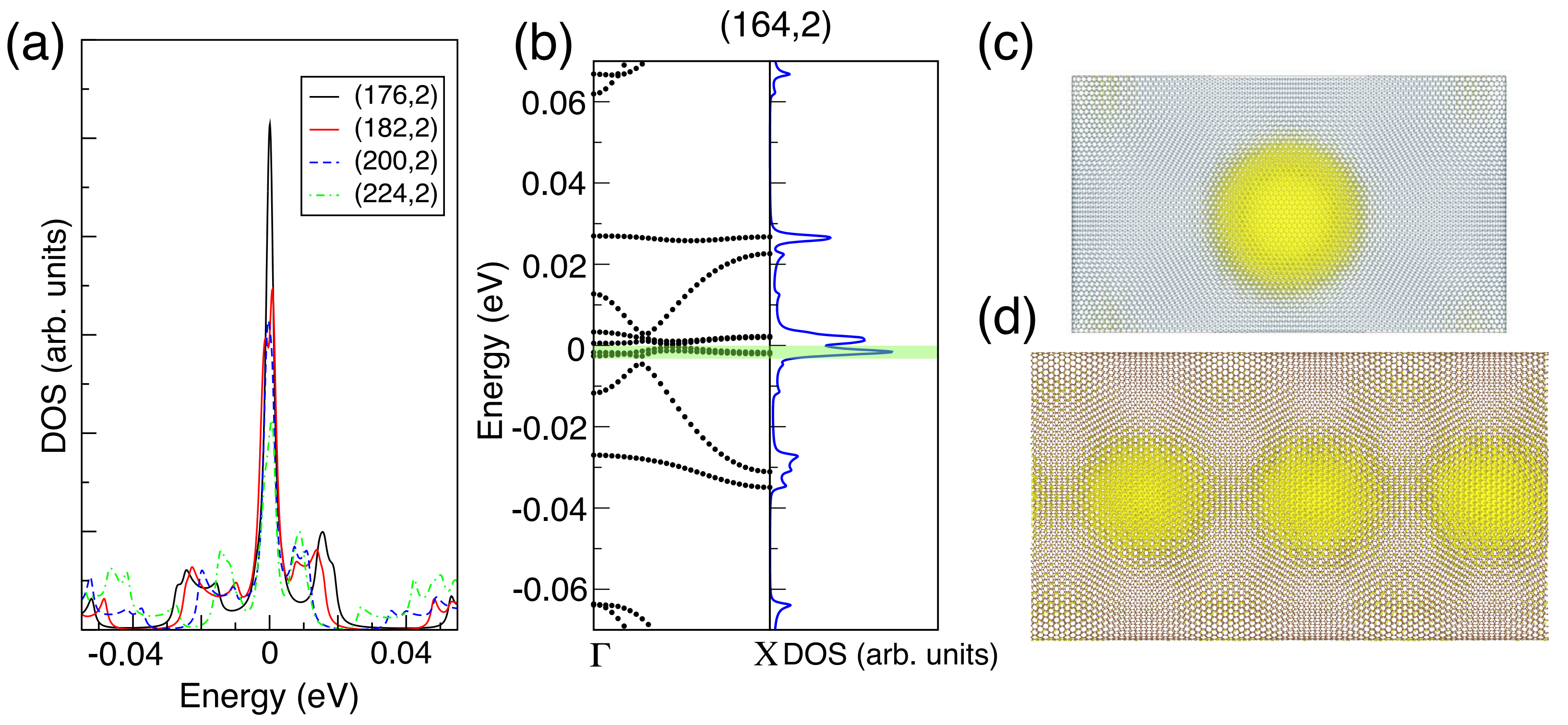


(176,2)
$\theta_M \sim 1.12°$

Conclusions

- Collapsed chiral CNTs meet all benchmarks for being the 1D analogues of TBG.
- Depending on the symmetries of the tube, different moiré patterns appear, yielding various band structures. There is always a group of flat bands, which are linked to highly localized states. The (176,2) is the most suited metallic CNT. For semiconducting CNTs, yet unknown.
- Potential plaftorm for further research on topology, superconductivity and many-body interactions.

3. Strongest or narrowest density of states



(a) Density of states for several metallic tubes. (b) Band structure and DOS for the (164,2) tube. Top views of a metallic (c) and semiconductor (d) tubes with the LDOS highlighted in color.

The strongest DOS is that of the (176,2) tube. LDOS shows highly localized states associated with flat bands in the AA region, as in TBG.

4. Indications of strongly correlated system

$U/t \gg 1, V/t \gg 1$

References

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