# ONE-DIMENSIONAL MOIRÉ SUPERLATTICES AND FLAT BANDS IN COLLAPSED CHIRAL CARBON NANOTUBES

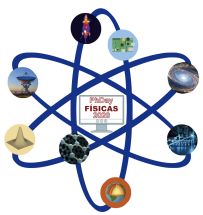
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PhDay 2020

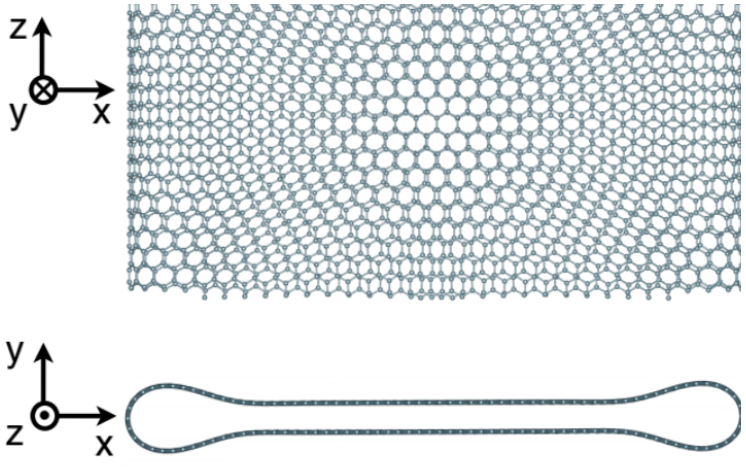




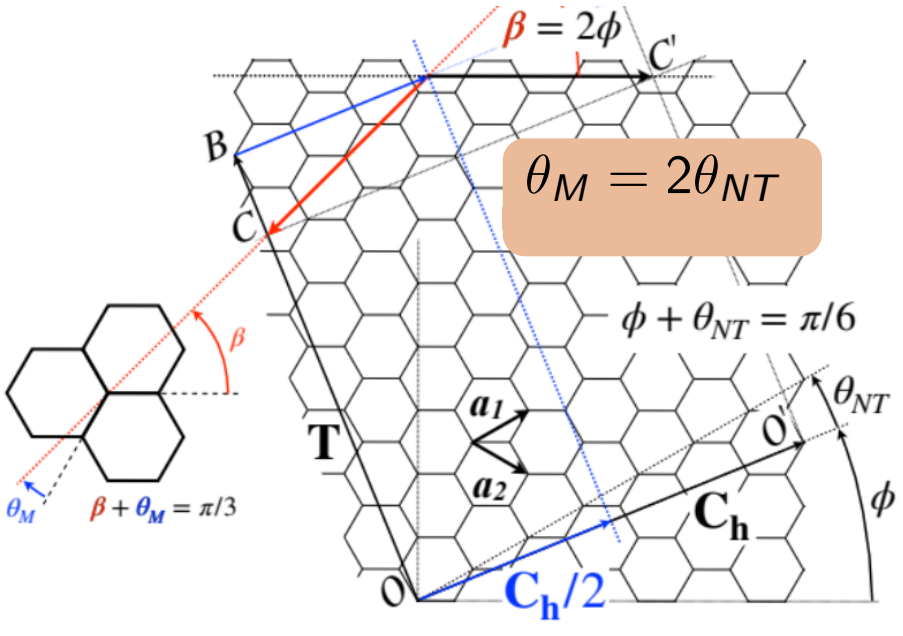



# SYSTEM GEOMETRY AND MOTIVATION

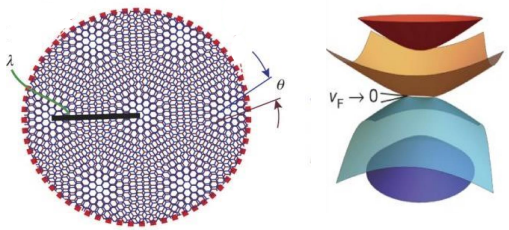
Cylindrical **chiral carbon nanotubes** (CNTs) can be **collapsed** via molecular dynamics and are proposed as a one-dimensional analogue to well-known **twisted bilayer graphene** (TBG), which yields moiré patterns, superconductivity and many-body electronic correlations.




Arroyo-Gascón, O., Fernández-Perea, R., Suárez Morell, E., Cabrillo, C., and Chico, L. Nano Lett. doi: 10.1021/acs.nanolett.0c03091 (2020)




$\theta_{TBG} \sim 1.1°$



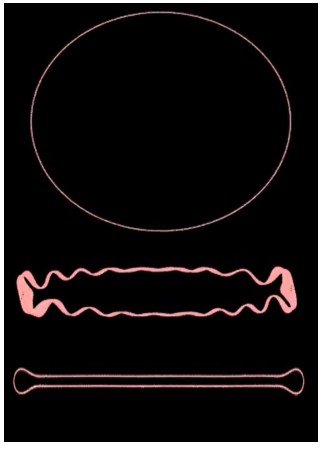

Cao, Y., Fatemi, V., Demir, A. et al. Nature **556**, 80–84 (2018)

# COMPUTATIONAL APPROACH AND METHODS

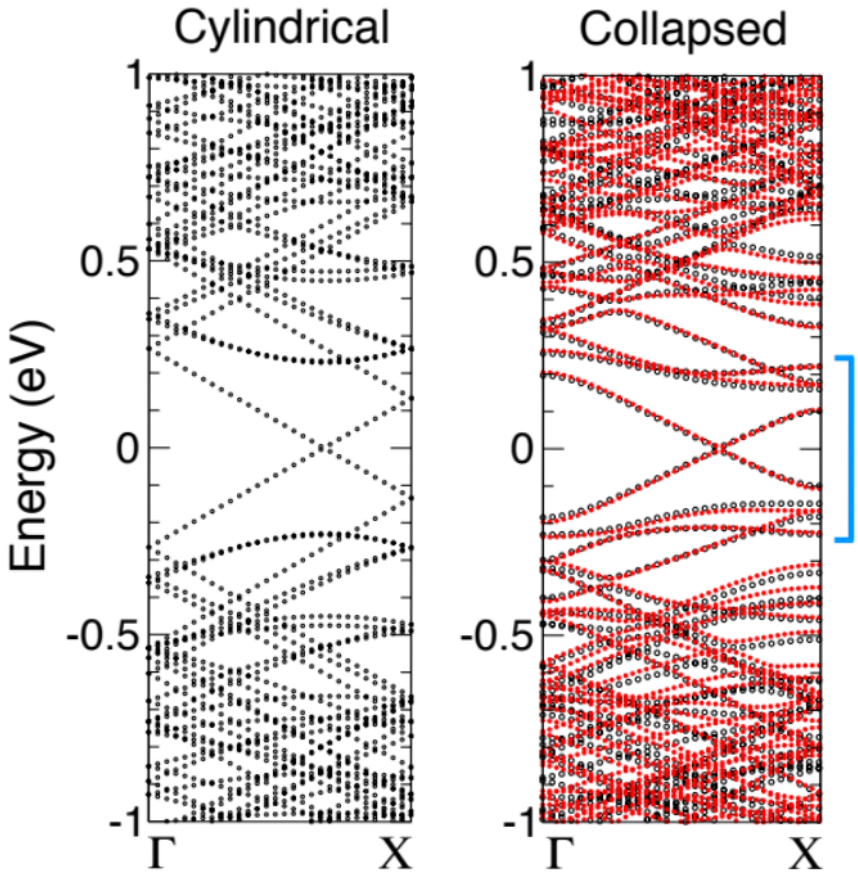
**Tight-binding hamiltonian:**

$$H = -\sum_{i,j} t(\mathbf{R}_i - \mathbf{R}_j) \, |\mathbf{R}_i\rangle \langle \mathbf{R}_j| + \text{H.c.}$$

Nam, N. N. T.; Koshino, M. Phys. Rev. B **96**, 075311 (2017)



Molecular dynamics



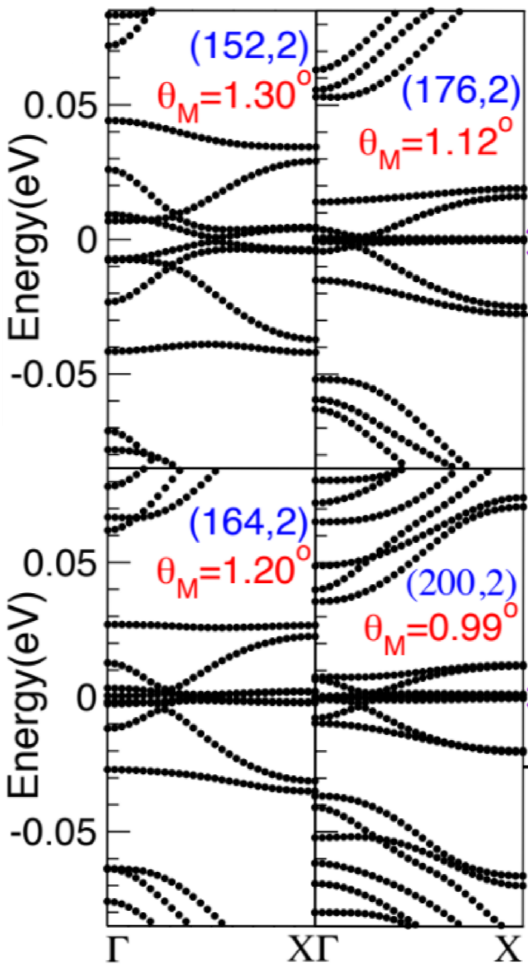

–TB
– DFT (SIESTA)

Model validated against DFT simulations for the $(62, 2)$ CNT (2648 atoms)

Arroyo-Gascón, O., F-P, R., SM, E., C, C., and C, L. Nano Lett. doi: 10.1021/acs.nanolett.0c03091 (2020)

# EVIDENCES OF MAGIC ANGLE PHYSICS

## 1. Flat bands and minimum bandwidth

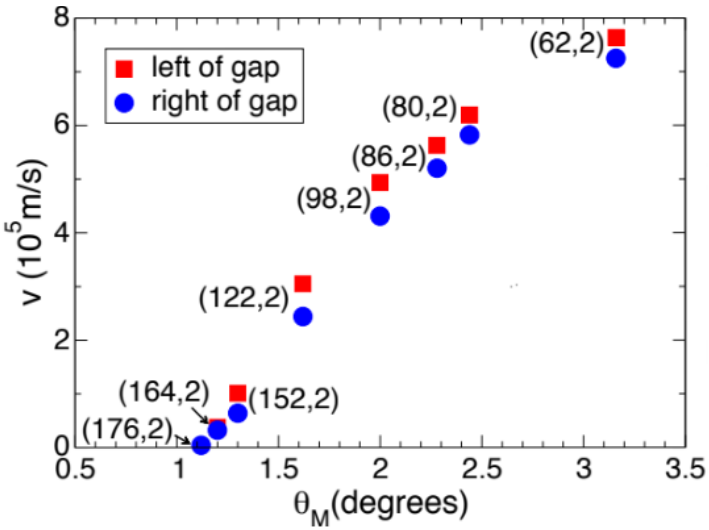


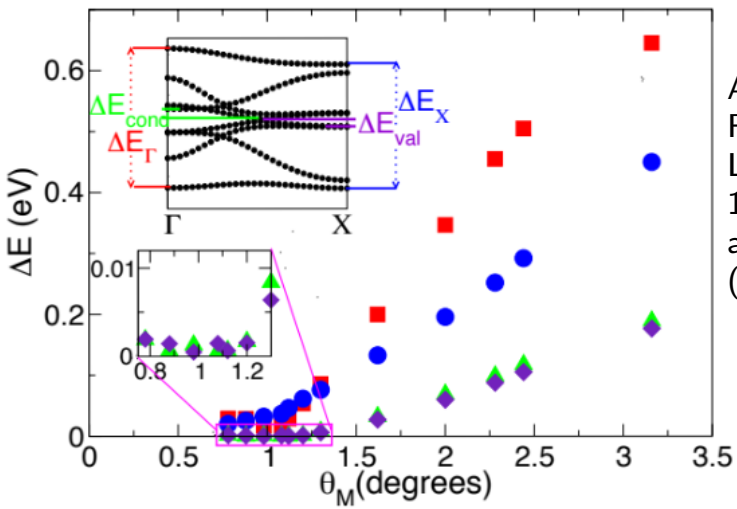

Central 8-band set and 2 central bands

(176, 2)

$\theta_M \sim 1.12°$

## 2. Velocity $v_F \sim 0$

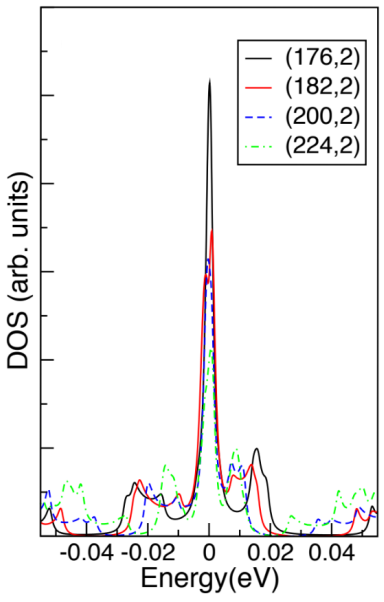


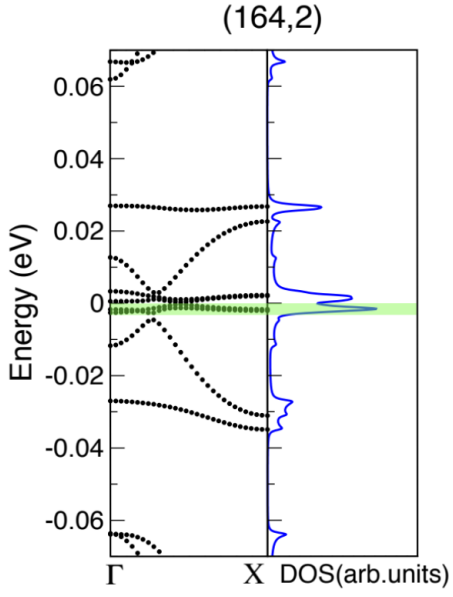

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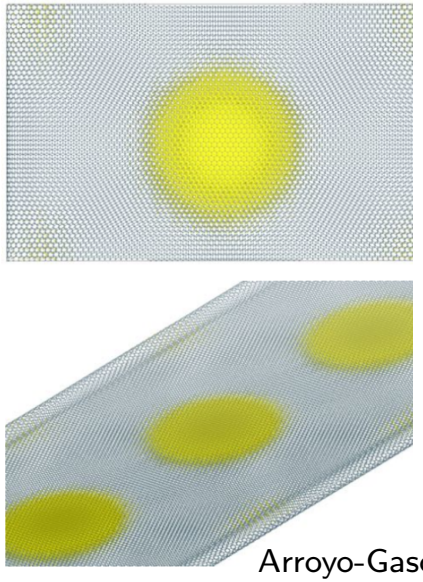
**3.** Strongest or narrowest density of states




Density of states (DOS)




Local density of states (LDOS)



States localized in the AA region as in TBG

$(176, 2)$

$\theta_M \sim 1.12^\circ$

Arroyo-Gascón, O., F-P, R., SM, E., C, C., and C, L. Nano Lett. doi: 10.1021/acs.nanolett.0c03091 (2020)

**4.** Indications of strongly correlated system: $U/t \gg 1$, $V/t \gg 1$