

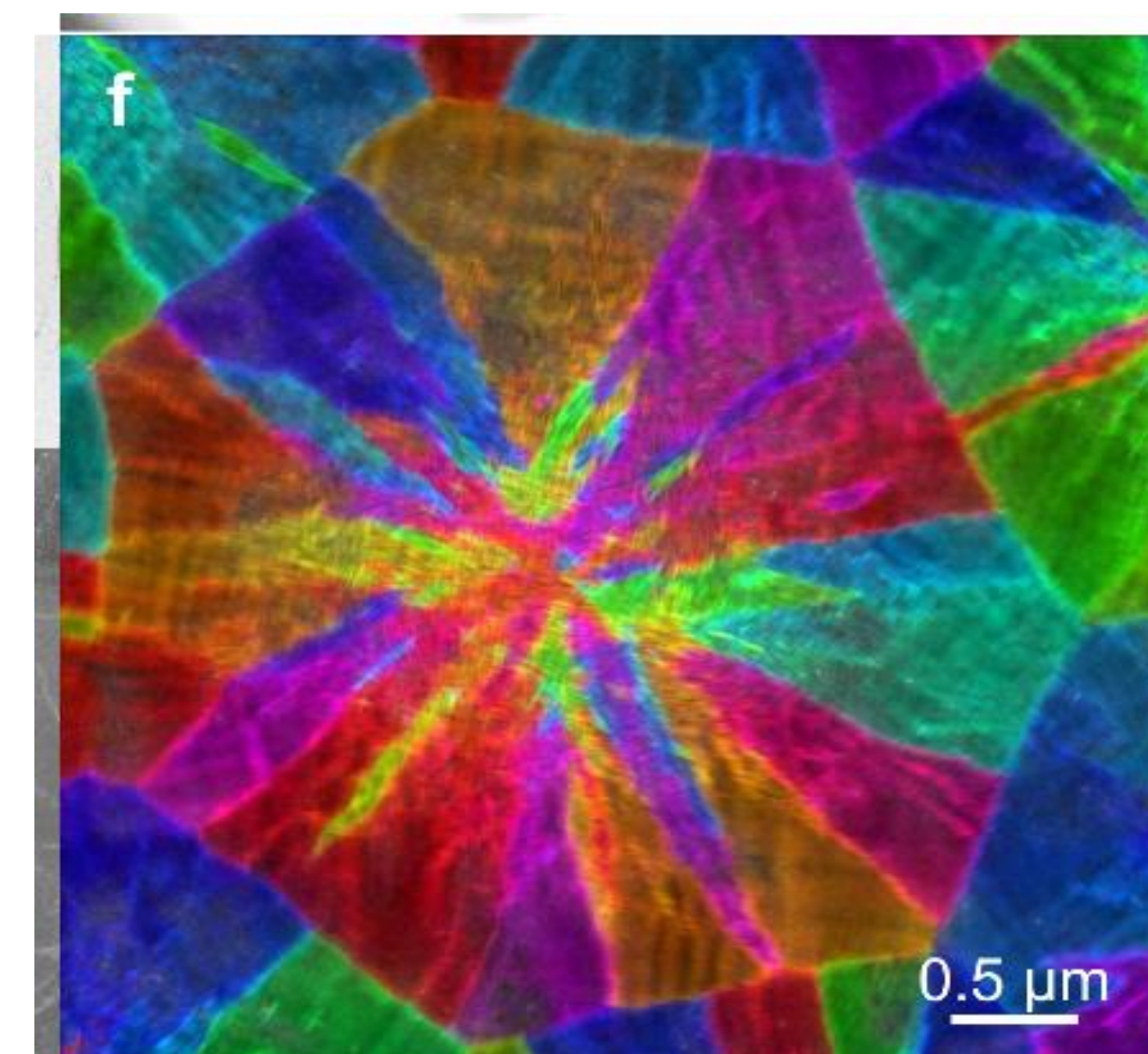
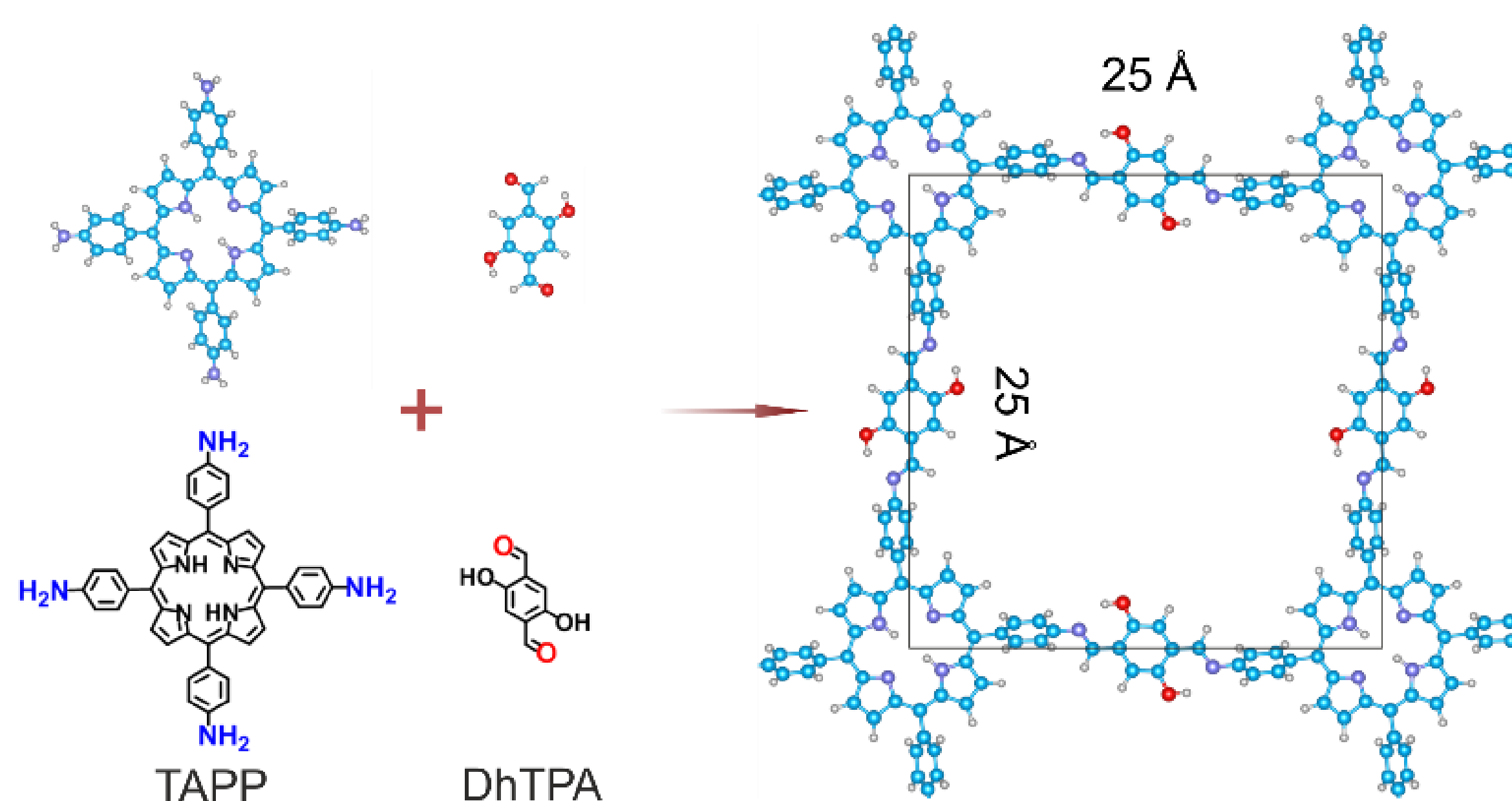
Structure of grain boundaries in a layer-stacked 2D polymer

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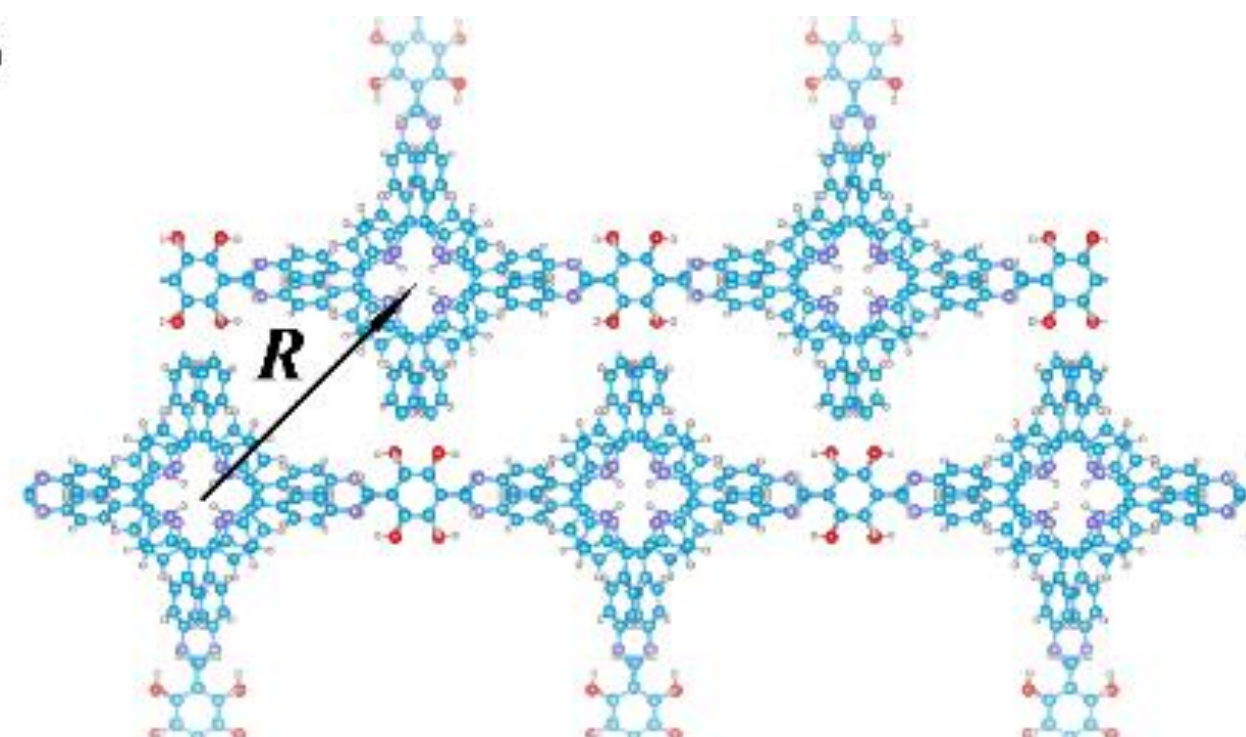
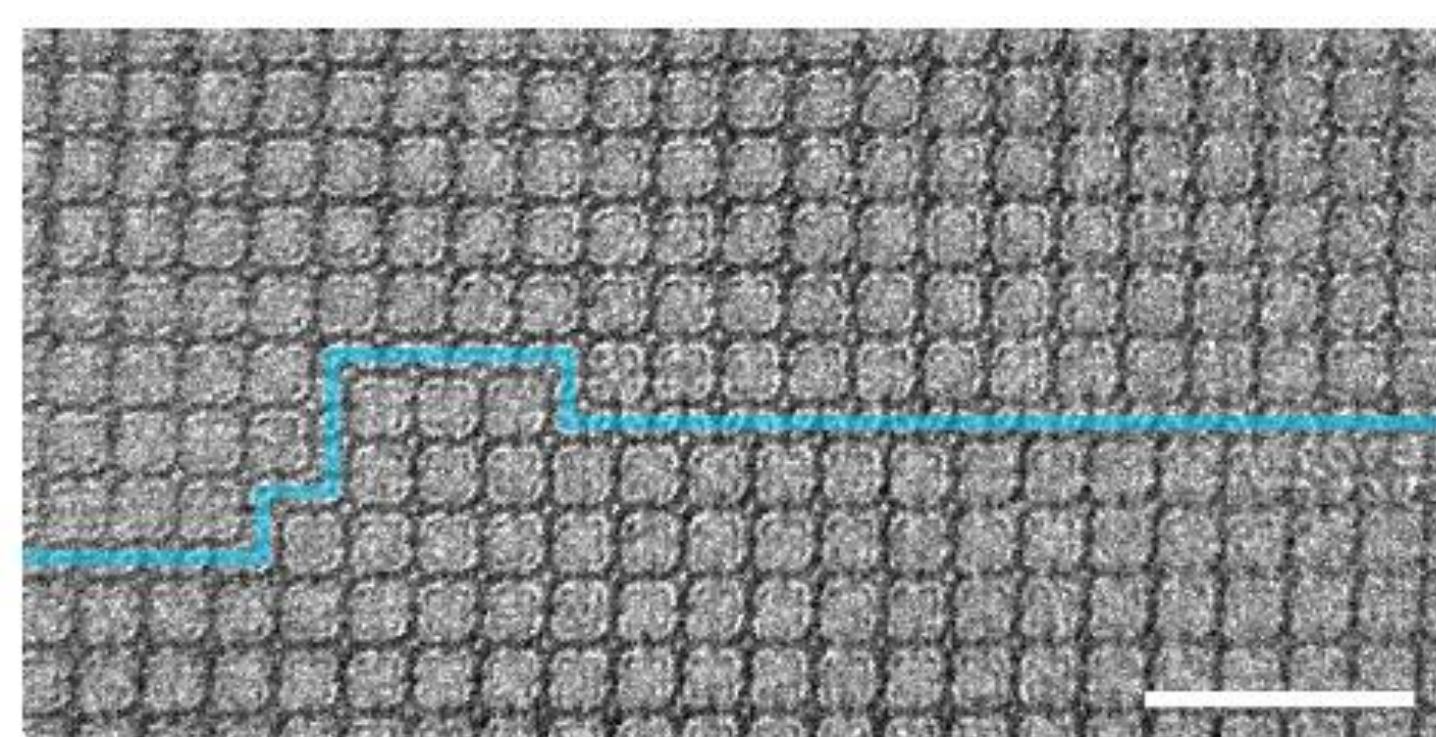
- Phase boundaries observed by AC-HRTEM in a layered 2D polyimine

- Unusual 3-7 membered rings boundary reconstruction observed at tilted boundaries

- Theoretical boundary models using DFTB show the boundary reconstruction is energetically viable

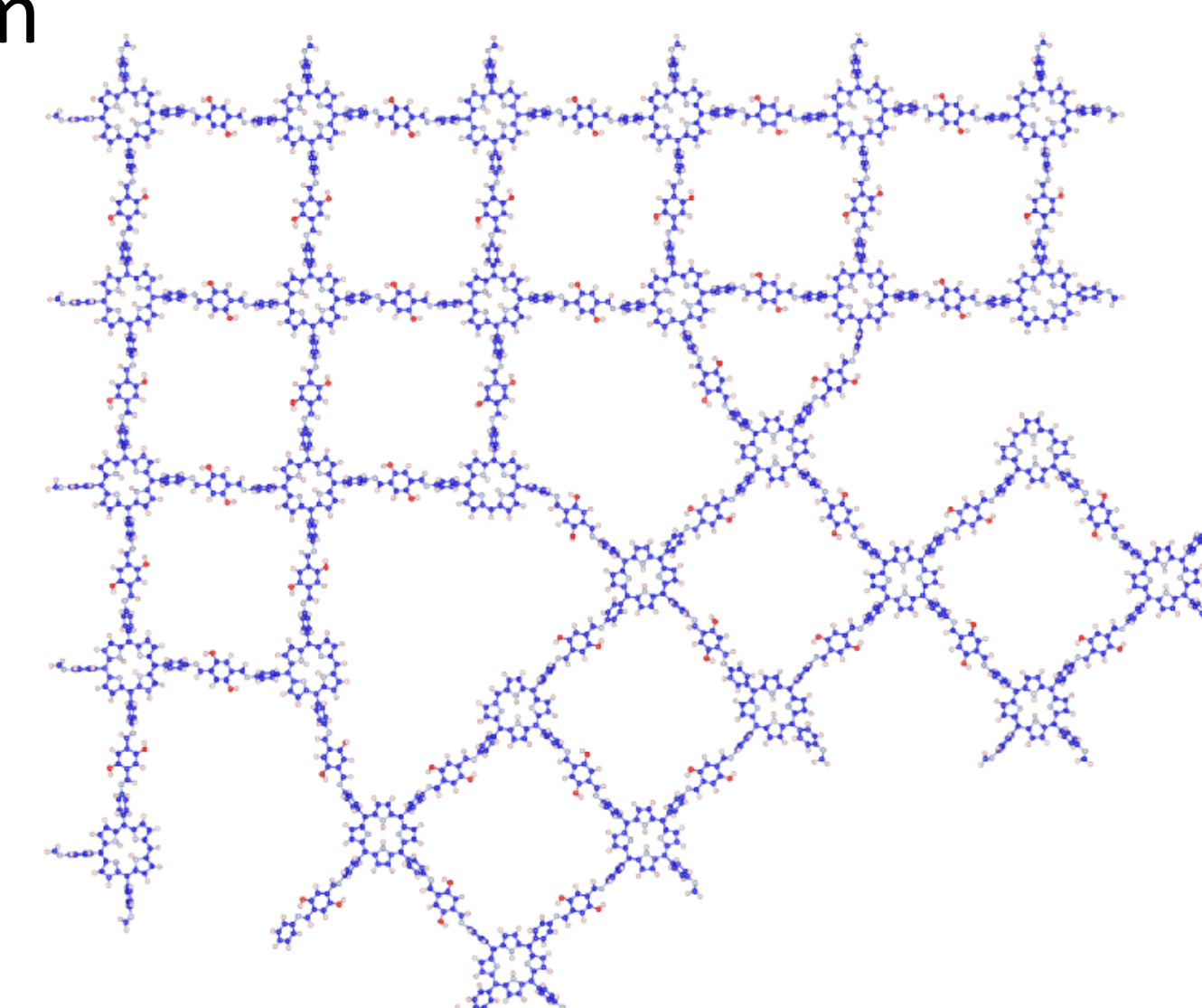


Antiphase boundaries



Theoretical Methods

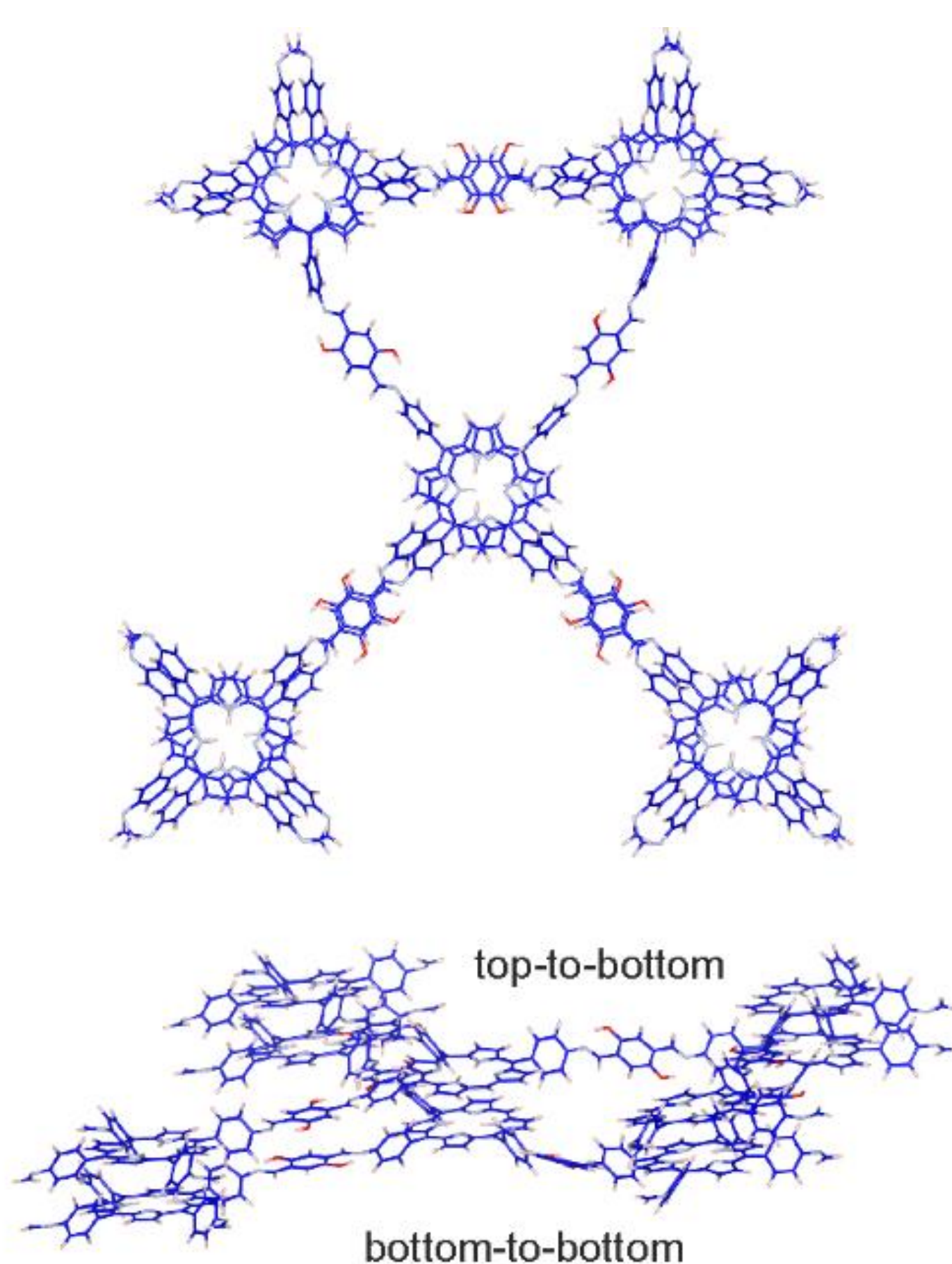
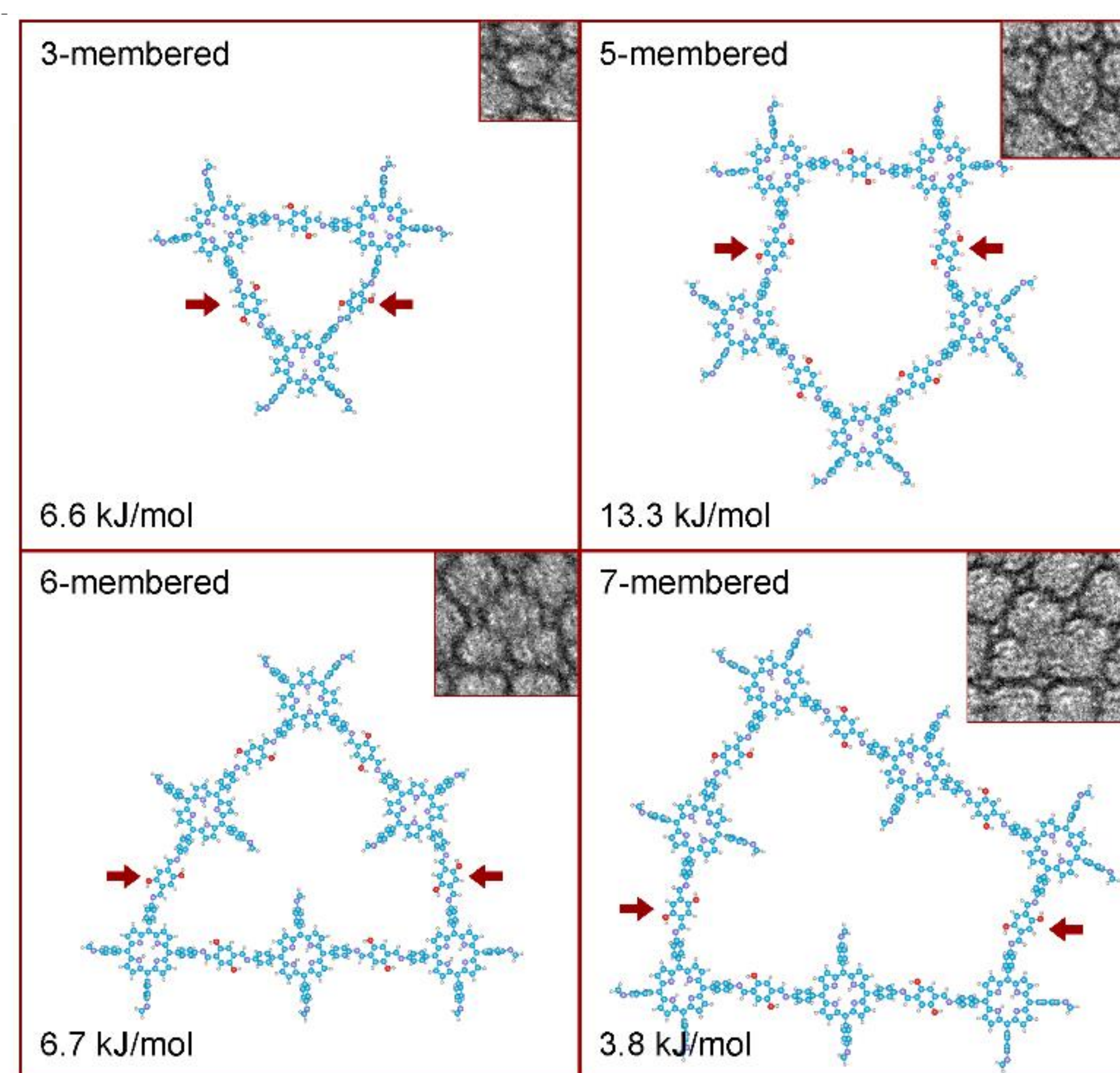
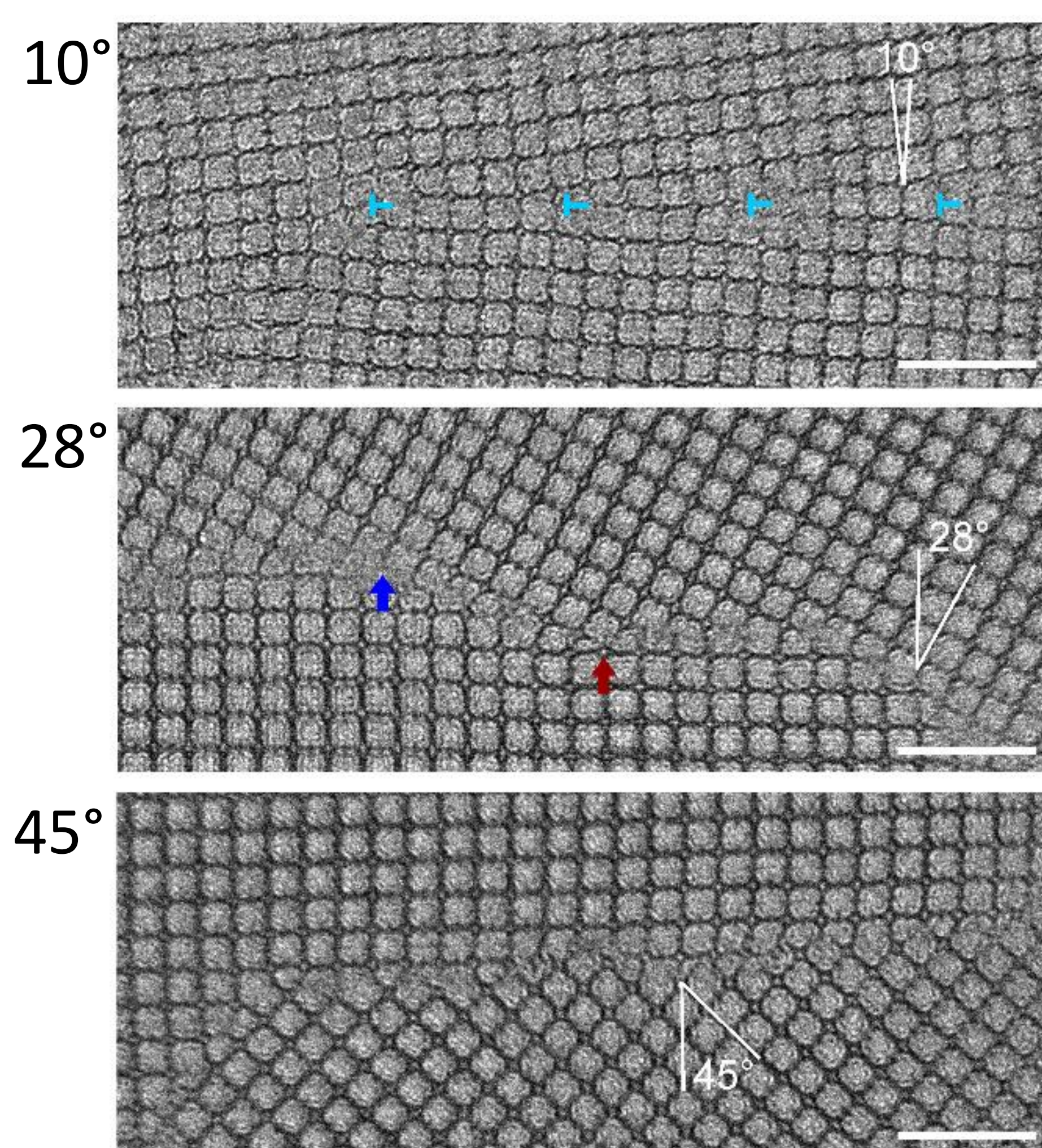
- SCC-DFTB in SCM (ADF) DFTB 2017 program
- mio-1-1 parameter set
- 3-7-membered ring models**
- Large scale boundary model created according 45° boundary observed by HRTEM
- Full optimization with UFF in SCM (ADF) UFF 2017



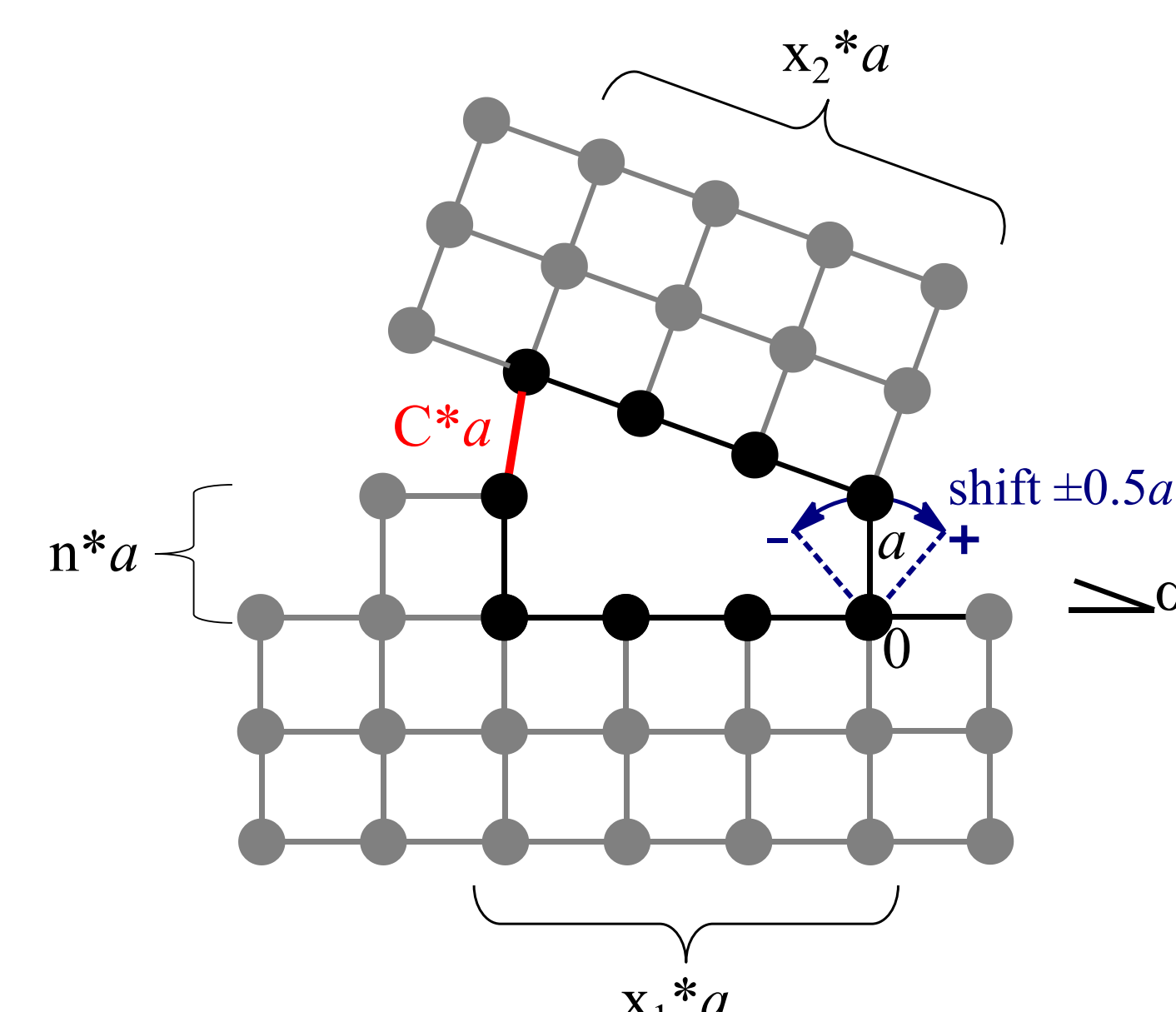
Presenter is a theoretician with only a limited knowledge of the HRTEM magic.

Tilted grain boundaries

- 10° occasional inter-grain reconnection
 - 7M rings visible
- 28° occasional inter-grain reconnection
 - 3, 5 and 6M rings observed
- 45° frequent inter-grain reconnection
 - 3, 5 and 6M rings observed
- Relative energy of inter-grain connections only 4-13 kJ/mol per "linker" compared to normal 4M ring, not prohibiting condensation reactions!



- In-plane reconnection and inter-layer connections have similar energy
 - Reconstruction of misaligned grains not prohibited!
- Geometry analysis of square lattice reconstruction
 - Identification of all angles and shifts when 2 connections can form
 - Tilt under 20° -> prolonged "rings" with (6)8+ members
 - Tilt 20-40° -> 6 to 10M rings possible
 - Tilt 45° -> 3, 5 and 6M rings possible



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REFERENCES

Qi, H., Sahabudeen, H., Liang, B., Položij, M., Addicoat, M. A., Gorelik, T. E., ... & Kaiser, U. (2020). Near-atomic-scale observation of grain boundaries in a layer-stacked two-dimensional polymer. *Science advances*, 6(33), eabb5976.

