Electronic structure of low-angle grain boundaries in naphthalene

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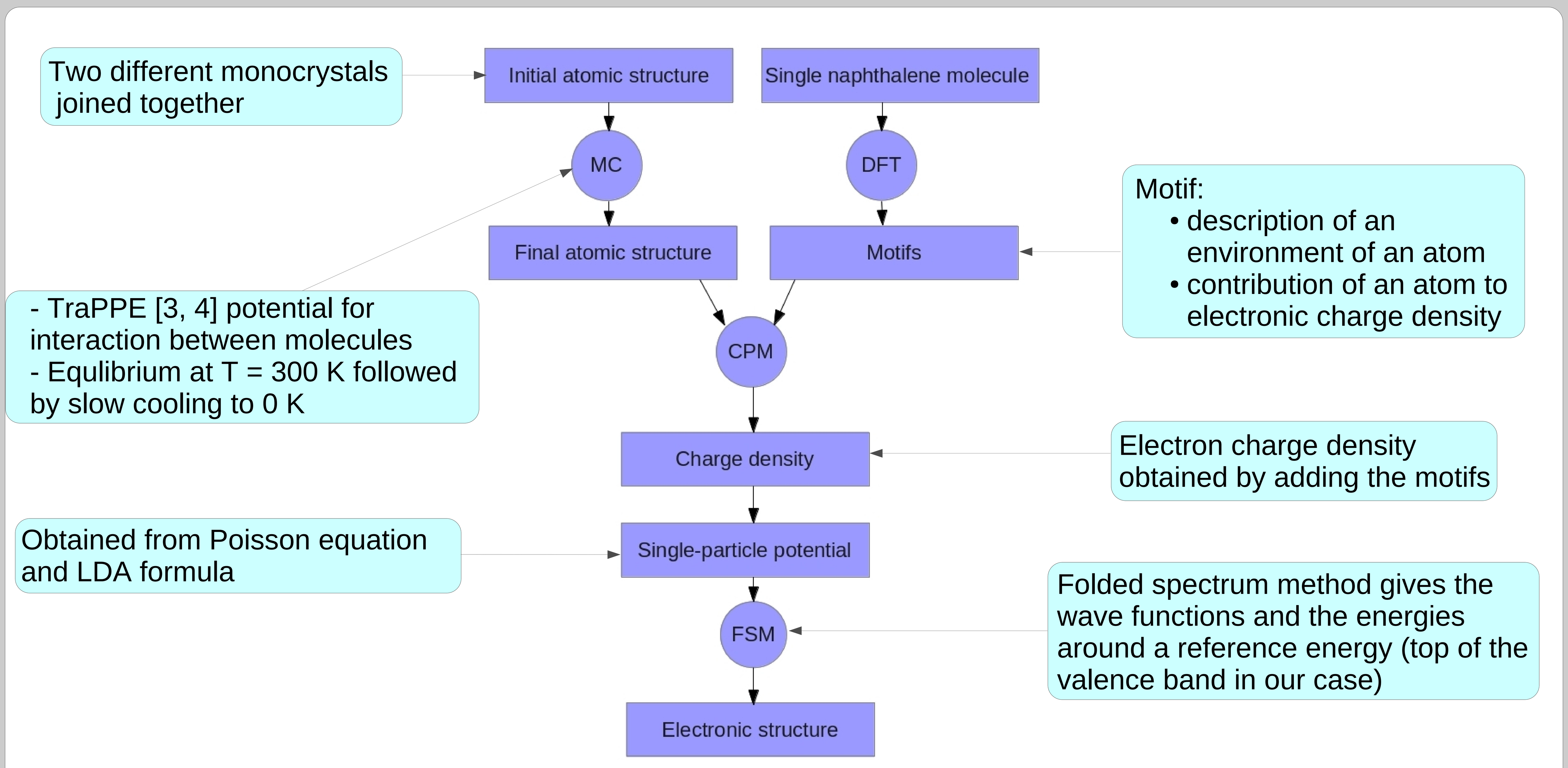
Introduction

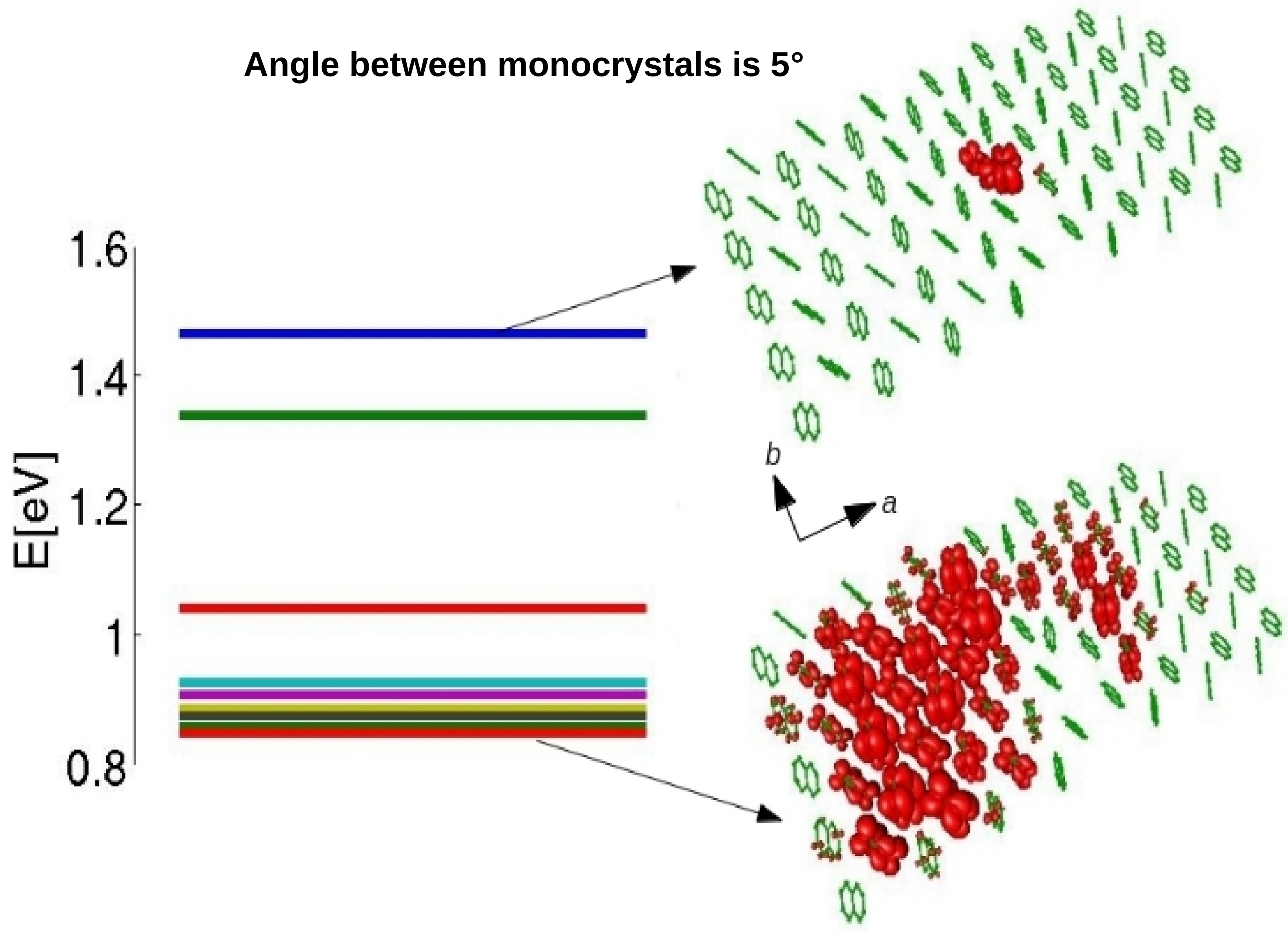
- Organic semiconductors are promising materials for LEDs, transistors and solar cells
- Crystalline organic semiconductors form polycrystals
- Grain boundaries:
  - contact surfaces between different monocrystals
  - produce trap states for charge carriers
  - affect the performance of the devices
- We present a method for investigation of the role of grain boundaries in organic semiconductors
- Atomic structure: Monte Carlo algorithm
- Electronic structure: charge patching method [1] and folded spectrum method [2]

Model description

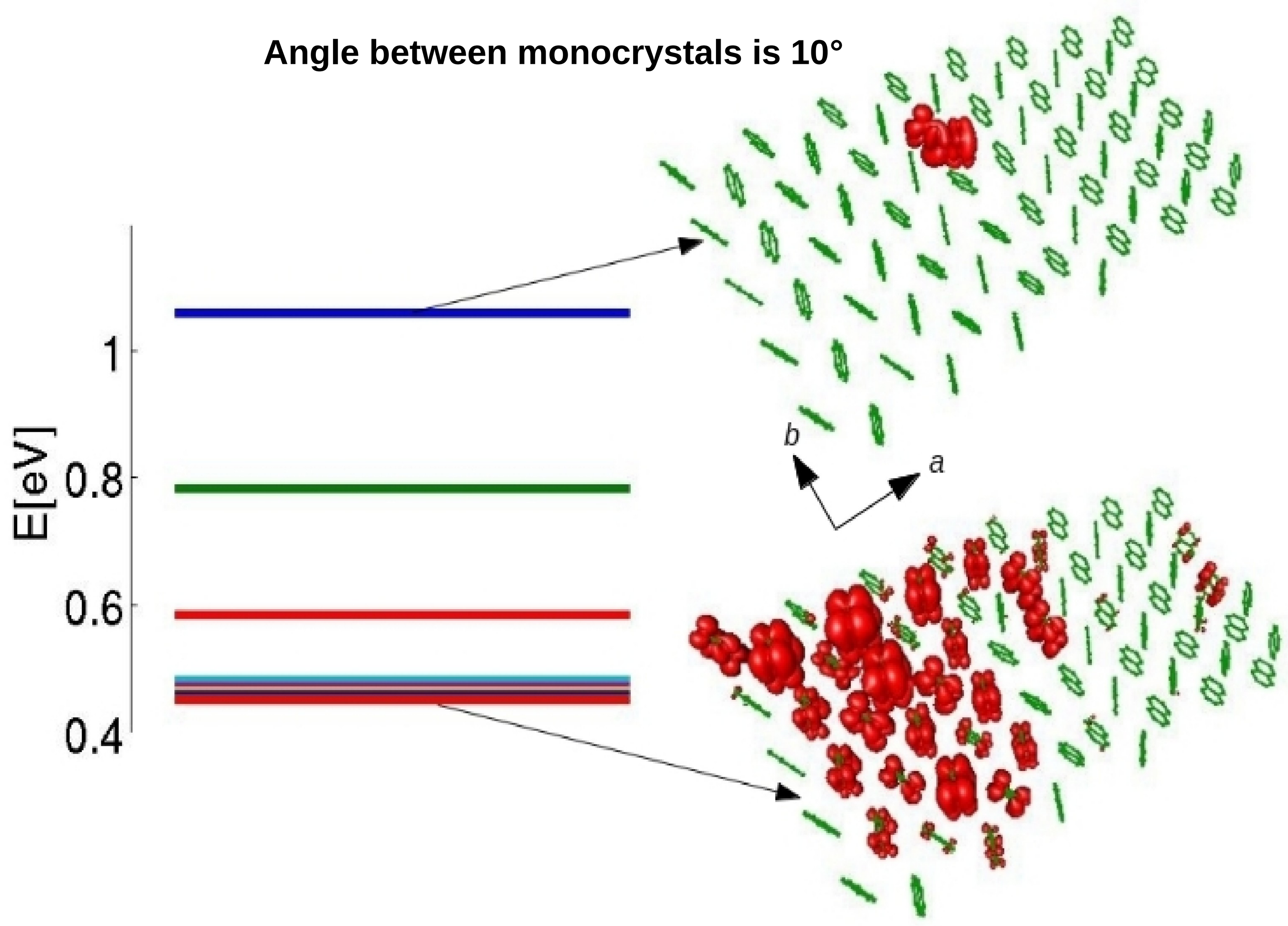


Results

Angle between monocrystals is 5°



Angle between monocrystals is 10°



Atomic structure:

- Molecules at the grain boundary slightly change their orientations
- Nearly unchanged away from the grain boundary

Electronic structure:

- Three states with energies significantly higher than the other energies
- Wave functions of these states are localized on two molecules on the grain boundary with smallest mutual distances
- Remaining states are mostly delocalized

Discussion

- Grain boundaries in organic polycrystals:
  - have small impact on atomic structure
  - introduce localized states in the energy band gap of a material
- Localized states at the grain boundary are trap states for charge carriers
- In the devices which operate in low carrier concentration regime, such as LEDs and solar cells, traps reduce carrier mobility
- Traps broaden absorption and emission spectrum

References:

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[2] A. Canning, L.Wang, A. Williamson, A. Zunger, J. Comp. Phys. **160,** 29 (2000)
[3] M. G. Martin, J. I. Siepmann, J. Phys. Chem. **B** 102, 2569 (1998)
[4] C. D. Wick, M. G. Martin, J. I. Siepmann, J. Phys. Chem. **B** **104**, 8008 (2000)

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SEVENTH FRAMEWORK PROGRAMME