Simulations of electronic states at grain boundaries in polycrystalline naphthalene

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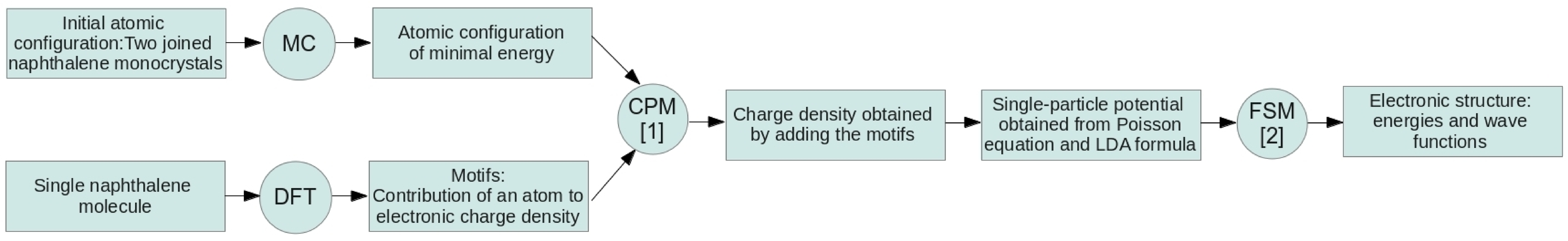
Introduction

- Organic semiconductors are promising materials for LEDs, transistors and solar cells.
- Crystalline organic semiconductors form polycrystals.
- Grain boundaries:
  - contact surface between monocrystals,
  - produce trap states for charge carriers,
  - affect the performance of the devices.

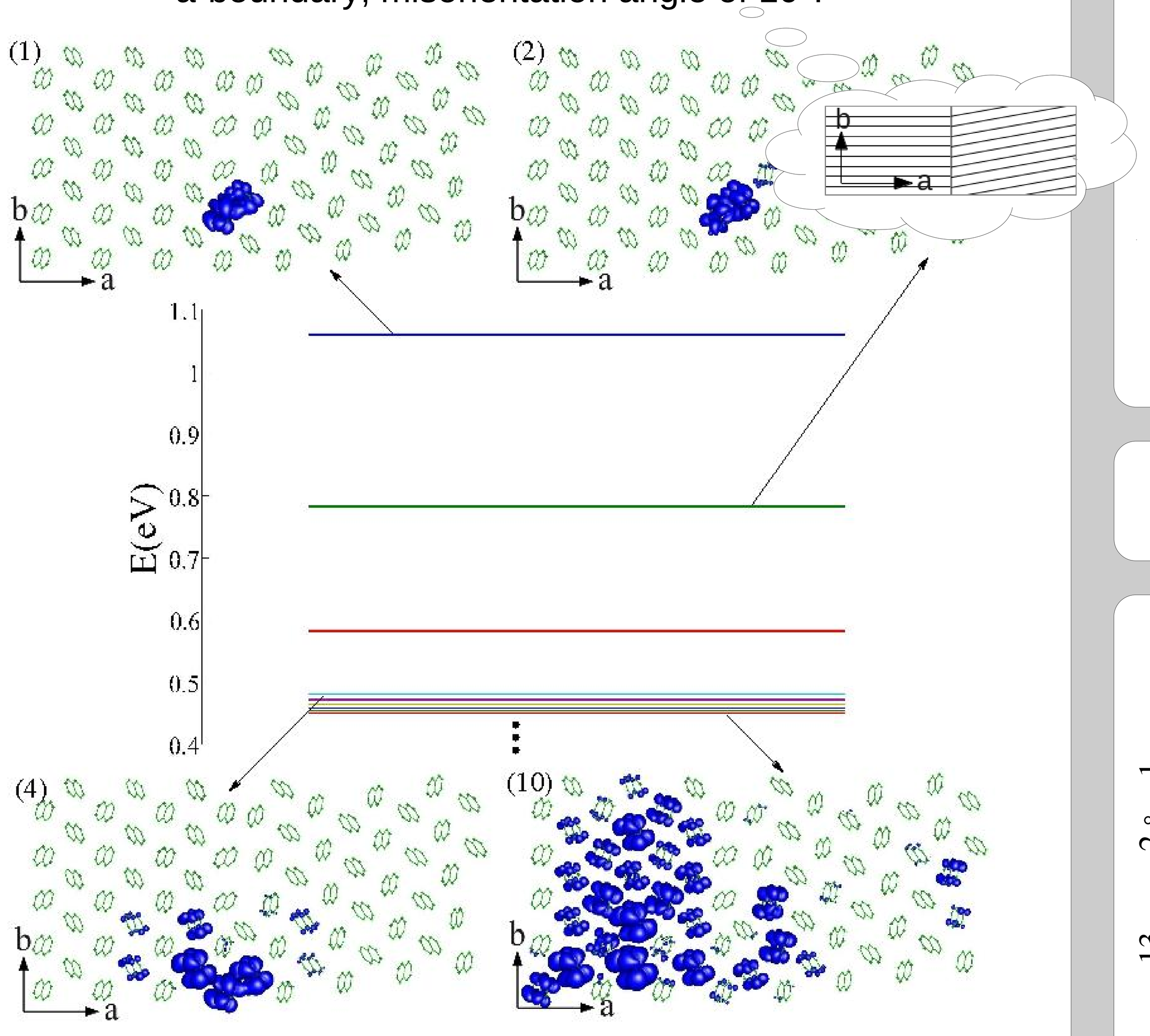
Method for electronic structure calculations



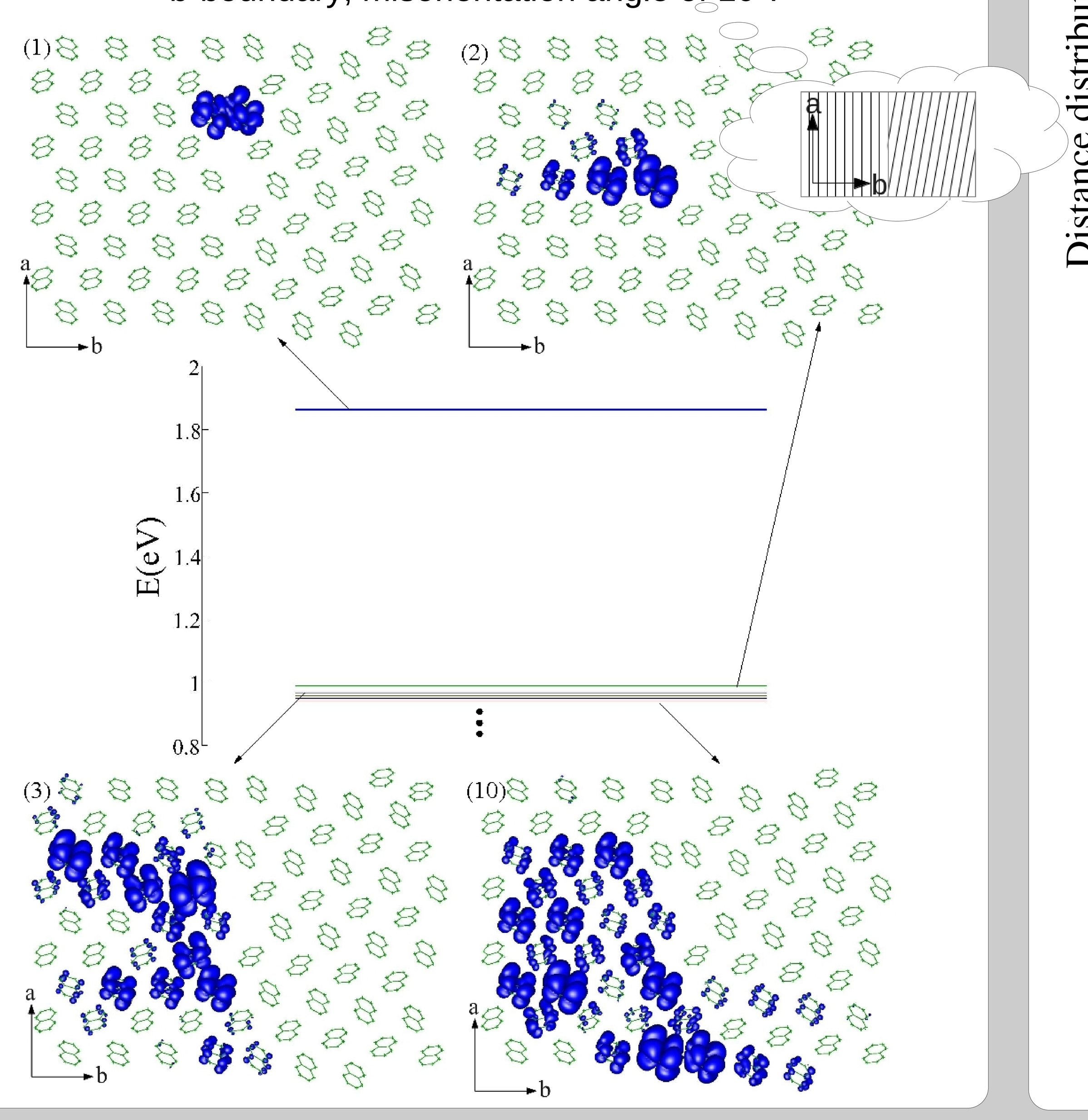
Wave functions at grain boundaries

Trap states at energies more than 0.1 eV above the valence band are localized on the molecule pairs (trapping pairs) at the grain boundary with mutual distance significantly smaller than the corresponding distance in the monocrystal.

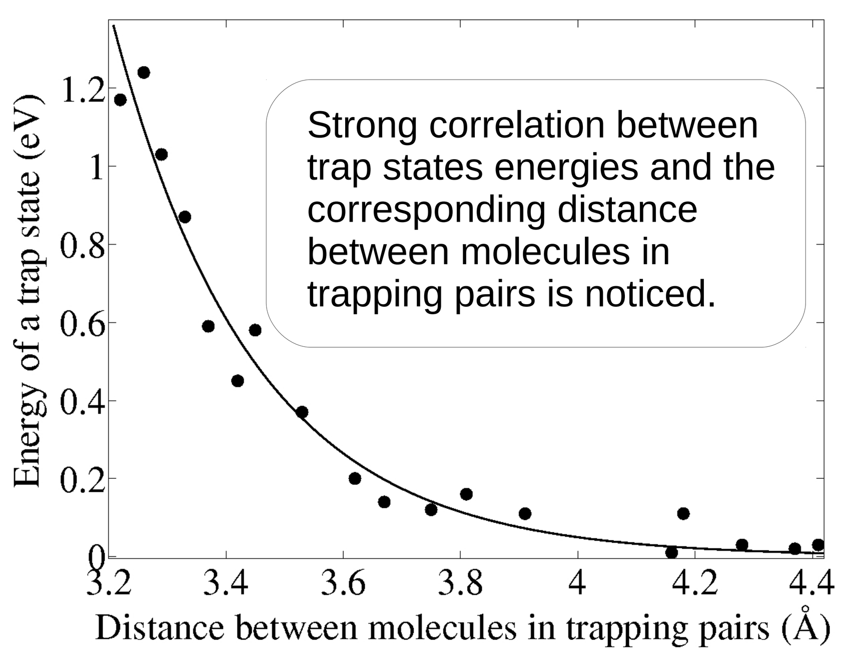
a-boundary, misorientation angle of 10º:

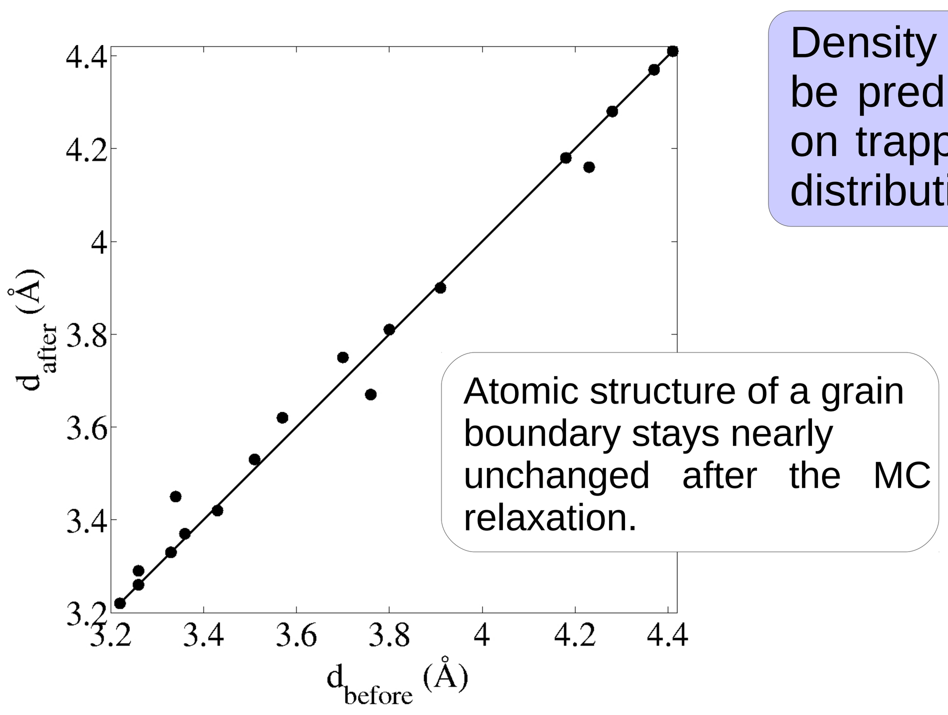


b-boundary, misorientation angle of 10º:



Method for density of trap states calculation



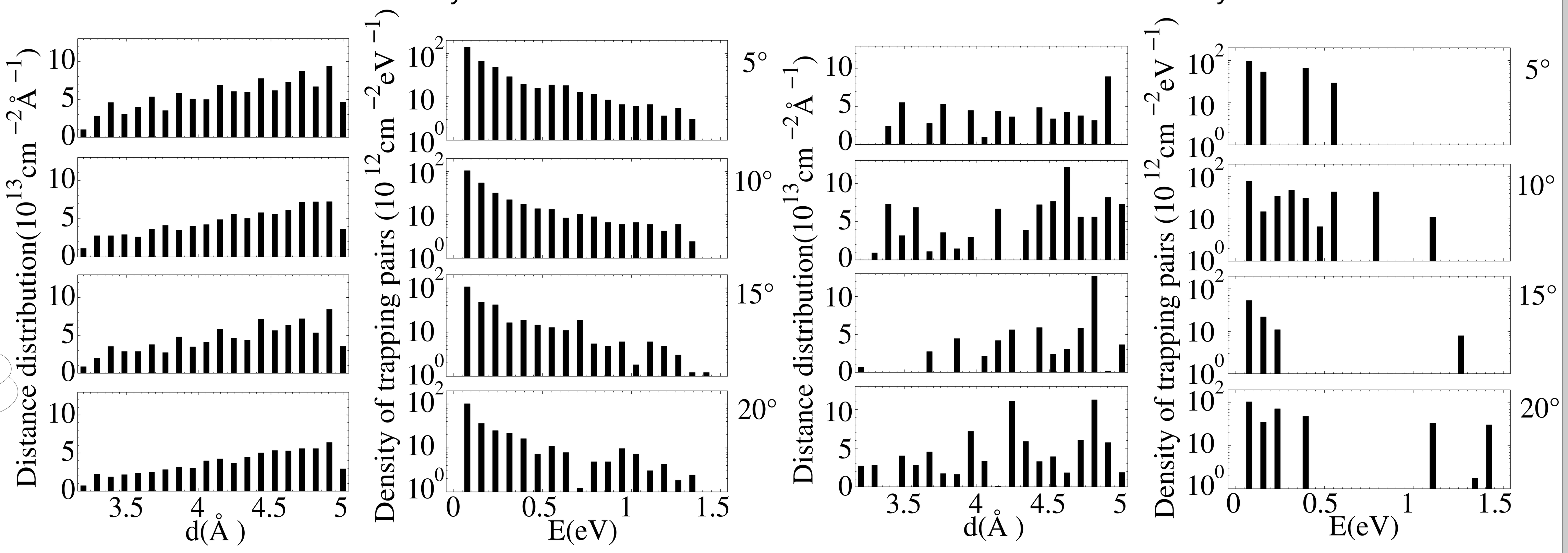


Density of trap states can be predicted solely based on trapping pairs distance distribution.

Density of trap states at grain boundaries

a-boundary:

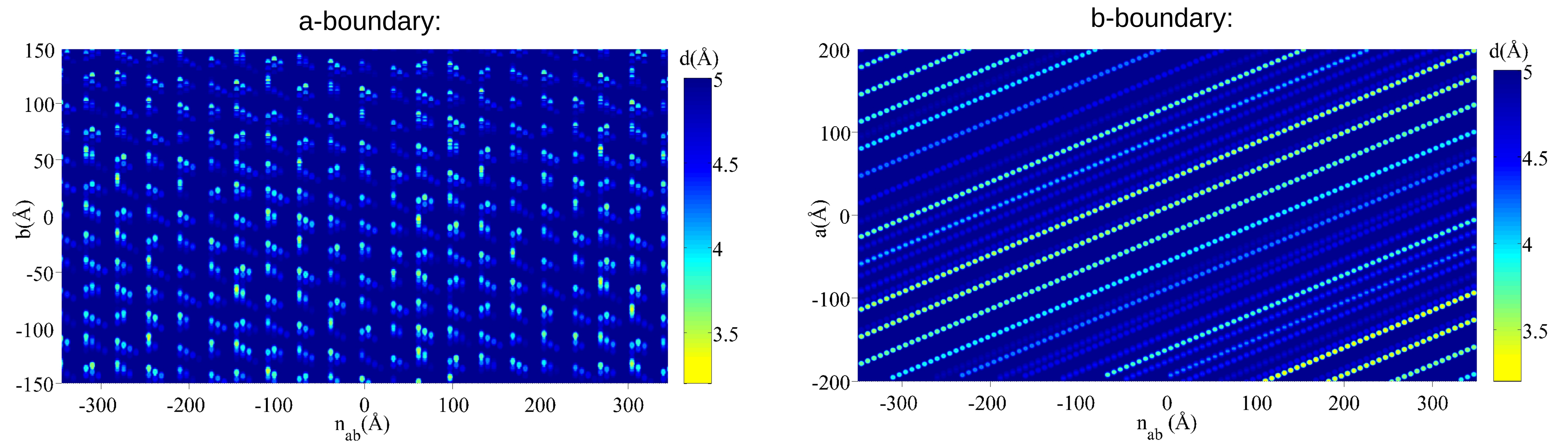
b-boundary:



Spatial trapping pairs distance distribution for misorientation angle of 10º:

a-boundary:

b-boundary:



Discussion

- Existence of grain boundary induced trap states in organic semiconductors is confirmed.
- For the first time, microscopic insight into the trap states is given.
- Method for easy density of trap states prediction is proposed.
- Estimated numbers of trap states per unit of boundary surface and volume are: 3×10^{13} cm^{-2} and 6.1×10^{17} cm^{-3}, respectively, which are of the same order of magnitude as experimental results for similar organic semiconductors. [3,4]
- Traps are expected to broaden the absorption and emission spectrum of the organic material in LEDs and solar cells.
- Charge carrier transport in transistors is expected to be strongly affected by the traps.

References:

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