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## Scenario

- Replacement of the fullerene derivative (PCBM) with carbon nanotubes (CNTs) as electron acceptor material in organic solar cells
- Nanoscale studies of the composites P3HT/CNTs to understand the physical interaction
- Improvement in the efficiency of the organic solar cells

## Goals

- UHV-STM study of the interaction and charge transfer between CNTs/conducting polymers
- Proper dispersion of the CNTs in order to form an ordered composite with conducting polymers
- Development and testing of a solar cell based on these composites

## Background

Many research efforts have been recently pursued in the field of thin film and organic photovoltaics, with the goal of reaching a power-conversion efficiency that will make such solar cells commercially viable. CNTs, because of their electrical and mechanical properties, are considered a valid material to replace the fullerene derivative (PCBM) in organic solar cells (OSCs). OSCs are expected to be commercialized soon.

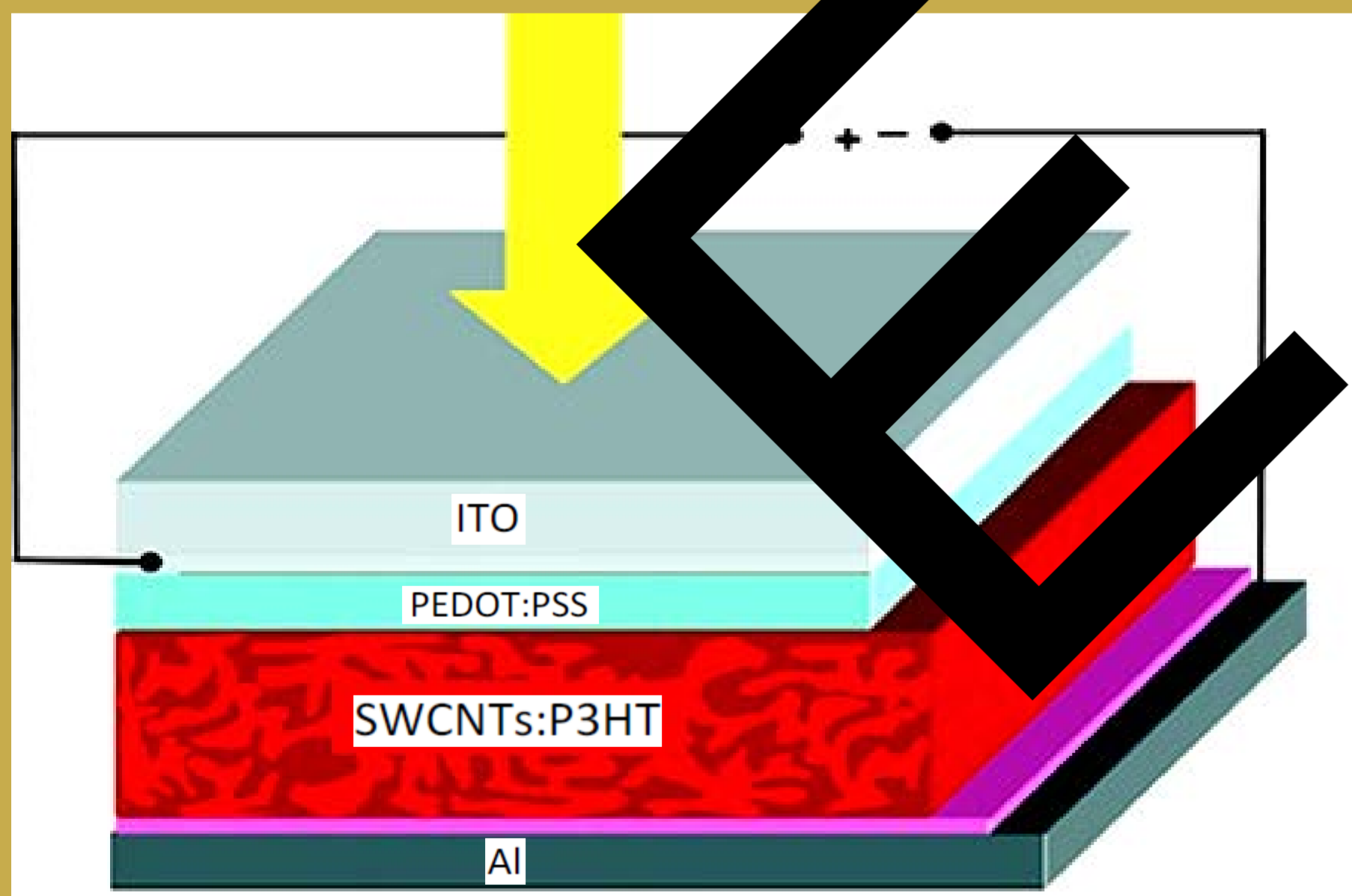
## OSCs

### Why CNTs in OSCs:

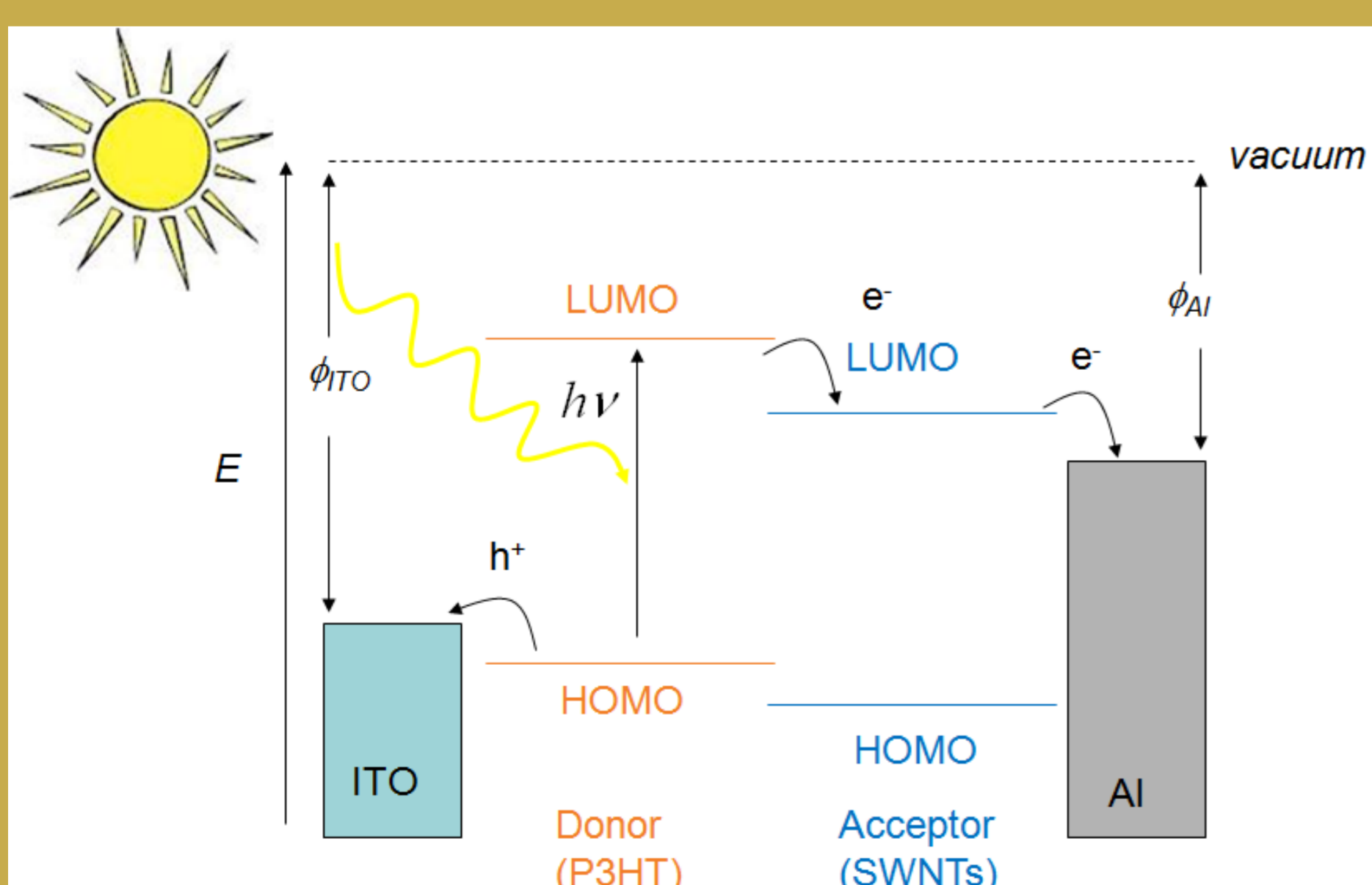
- Low percolation threshold
- High aspect ratio
- High conductivity
- Matching work function with fullerene derivative (PCBM)

### Bulk heterojunction OSCs:

- ITO glass
- PEDOT:PSS buffer layer (spin coating)
- Blend of SWCNTs:P3HT (spin coating)
- LiF buffer layer (thermal evaporation)
- Al cathode (thermal evaporation)

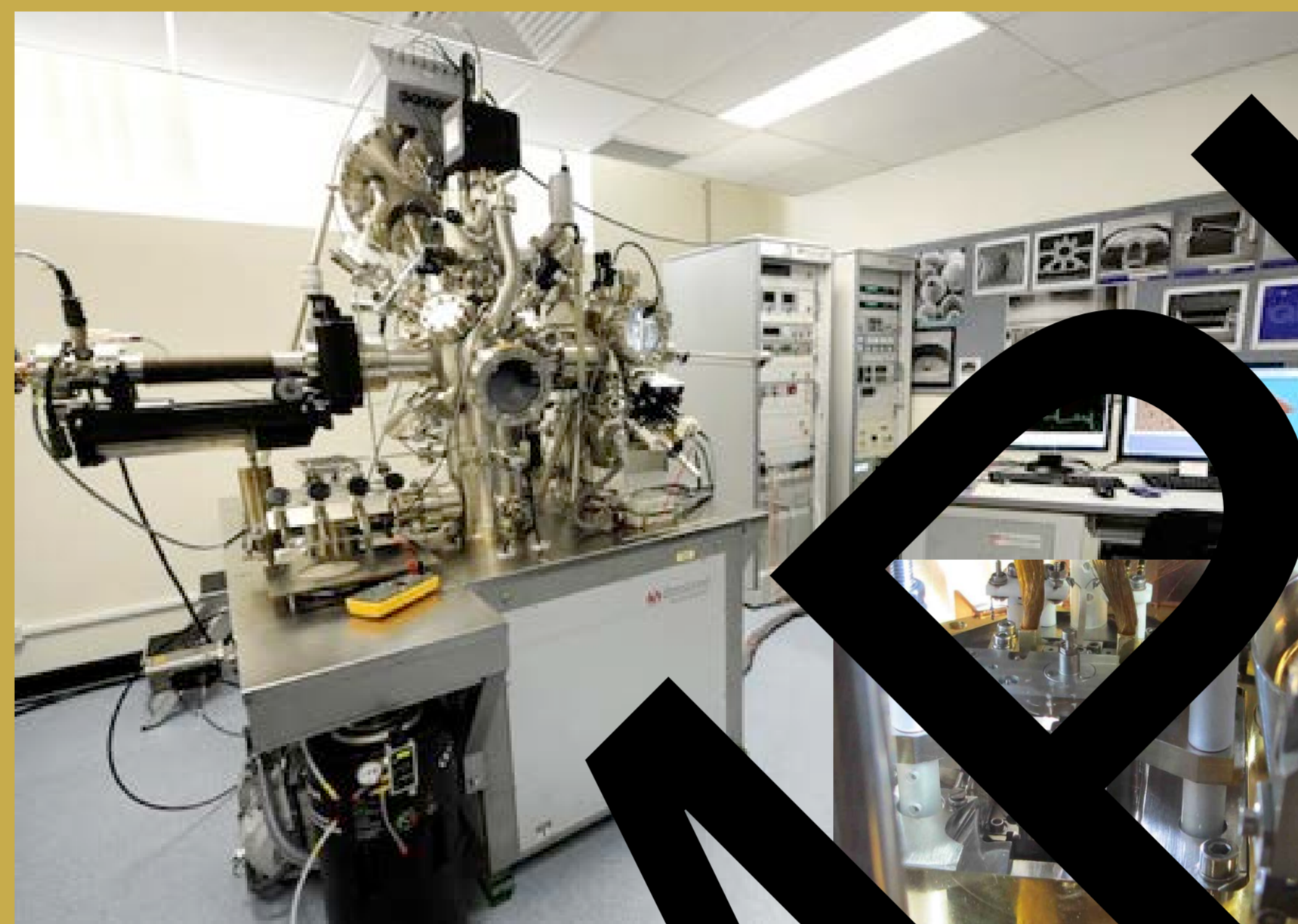


## Band diagram of a bulk heterojunction OSC

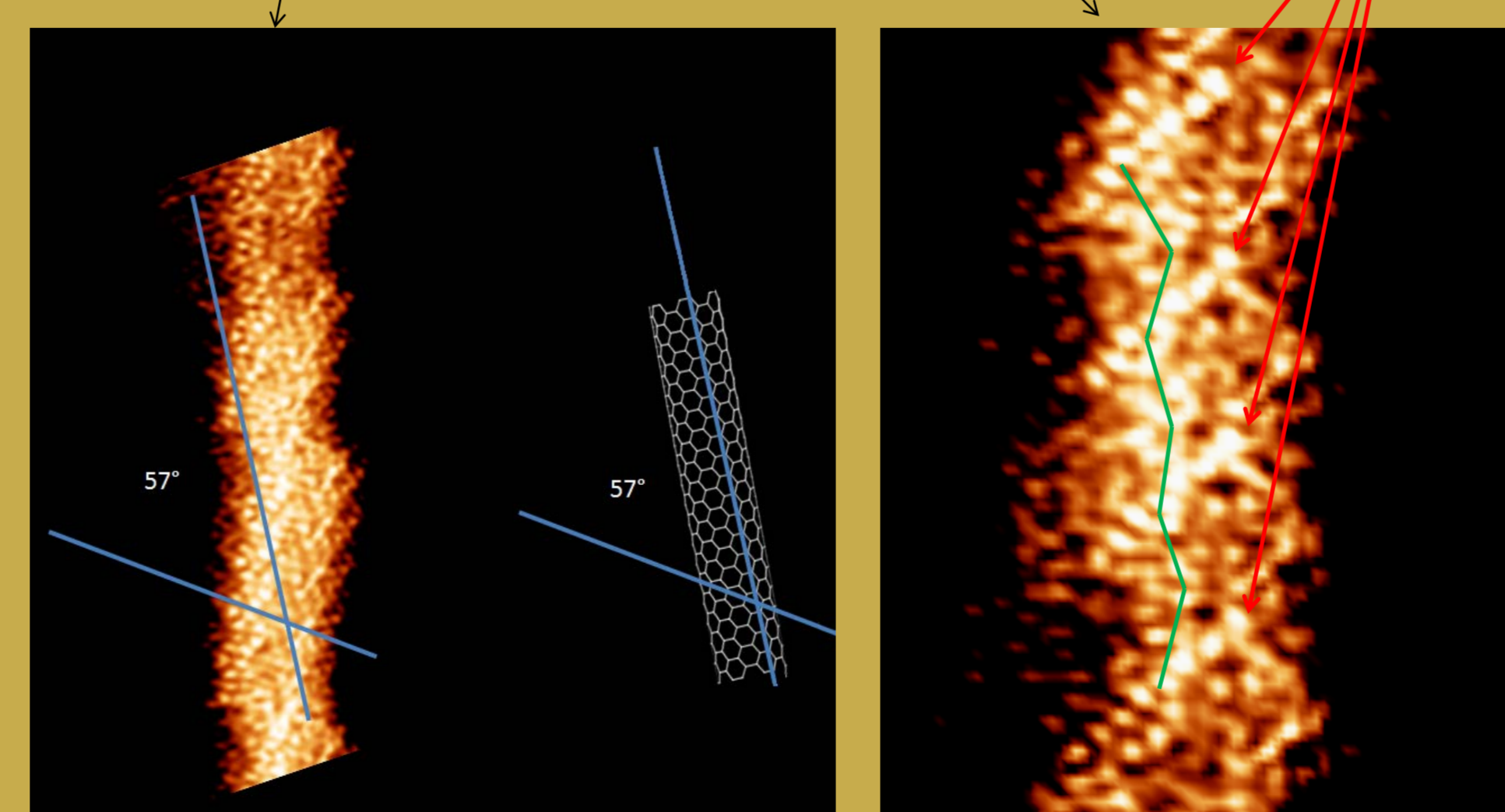
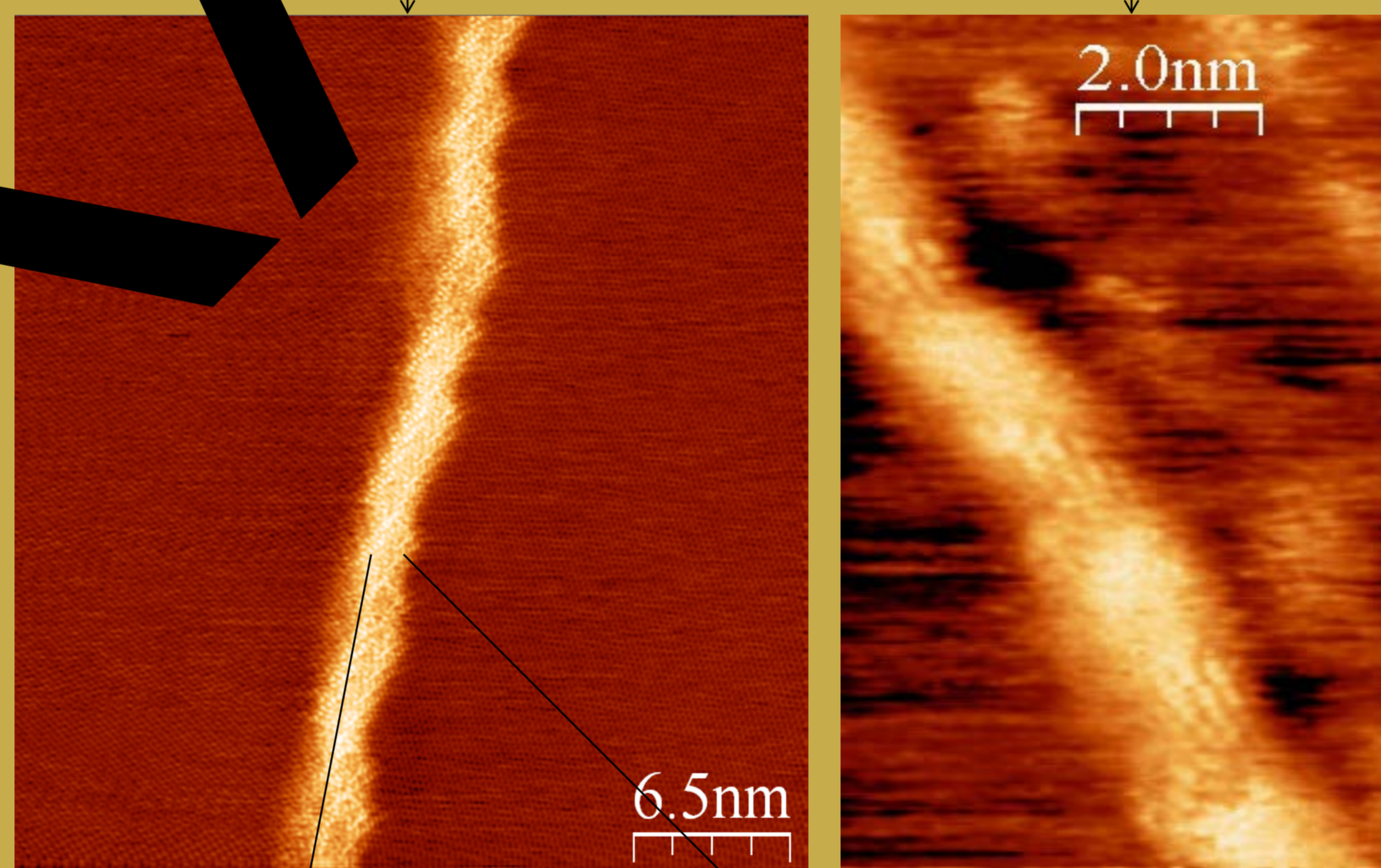


## Characterization

### Scanning Tunneling Microscopy at QUT



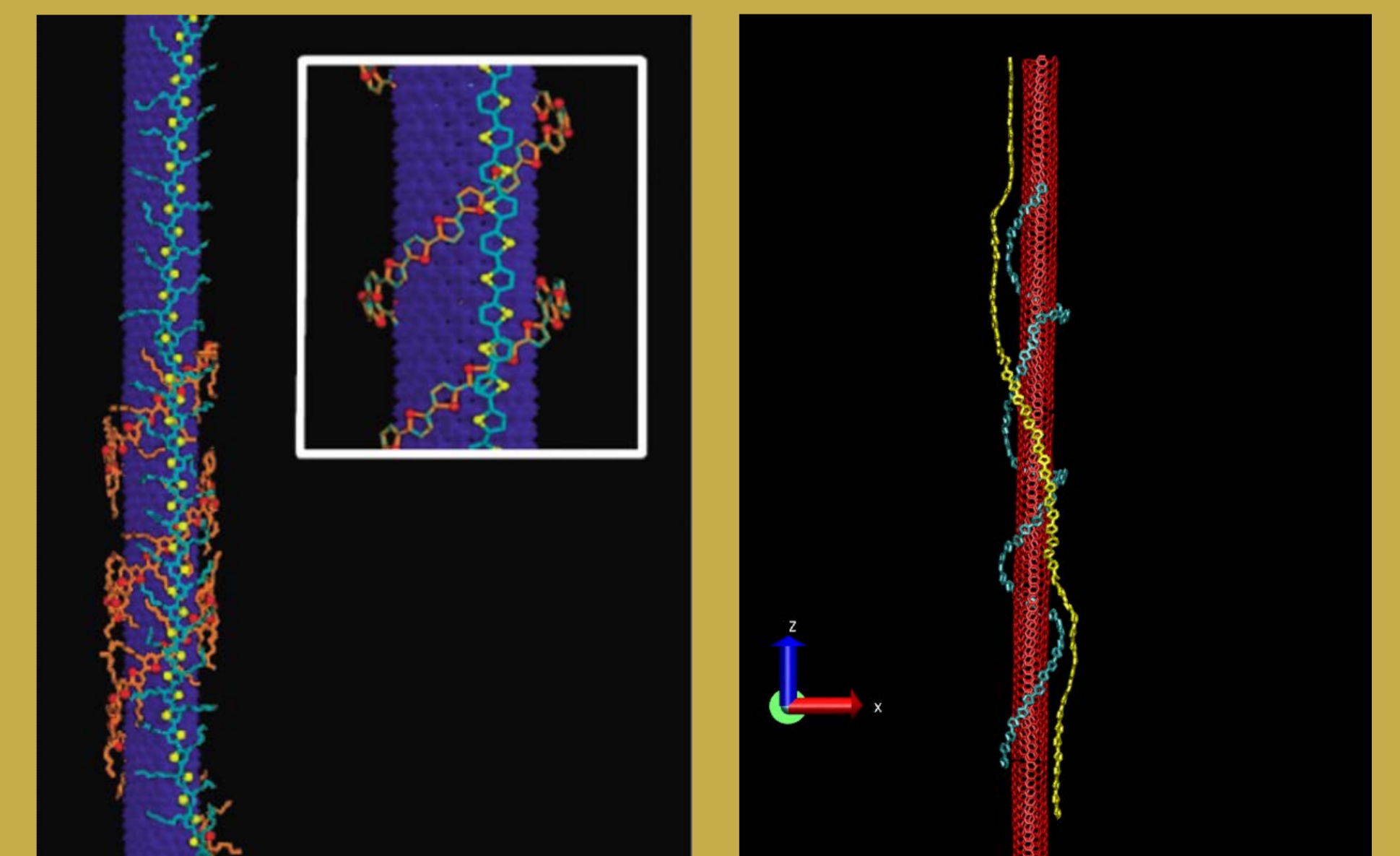
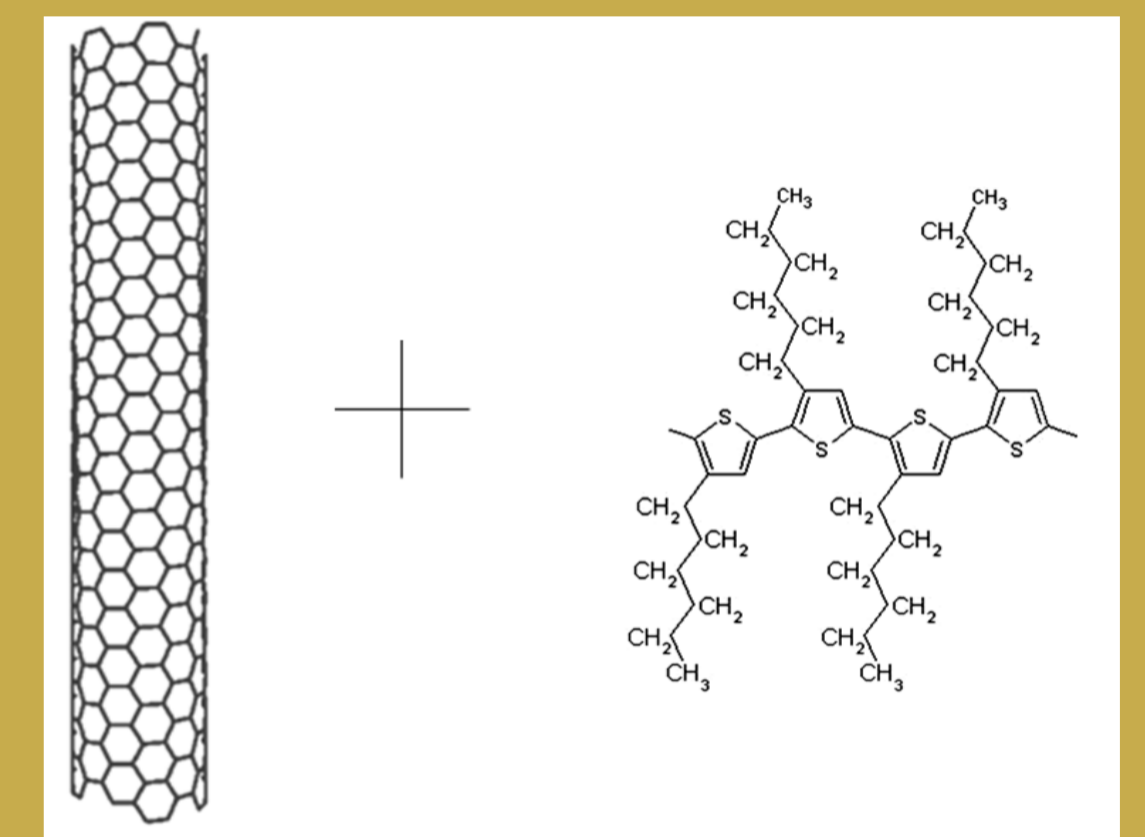
- Solution of SWCNTs (7,6)/rr-P3HT 10% wt in DCB
- Add cyclohexane 10% in volume to DCB
- Drop cast on HOPG + oven 65°C for 2h
- Solution of SWCNTs (15,0)/rr-P3HT 3% wt in DCB
- Drop cast on HOPG + oven 65°C for 2h



STM image confirms the presence of:  
 • SWCNT (7,6) through the chiral angle of 57°  
 • Longitudinal polymer backbone along the tube axis (in green) plus a wrapping polymer backbone (in red) is similar to the theoretical model

## Theoretical Model

- The SWCNT and the P3HT were investigated by Molecular Dynamics (MD) simulations and their interaction is described by the sum of two body Lennard Jones
- The equations of motion of atoms were integrated using the velocity Verlet algorithm



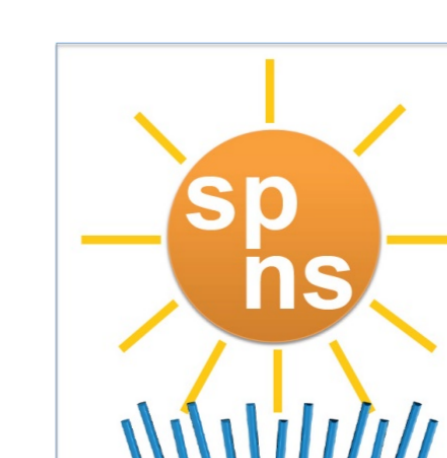
The model confirms the helical wrapping of the P3HT on SWCNT

## Conclusions

- STM studies of SWCNTs wrapped with polymers allow to understand the electronic properties of composites for solar cells

## Future Research

- Better dispersion of the composite in different solutions
- STM studies of the composite on Au substrate
- STM studies of SWCNTs/PCPDTBT composite
- Preparation and test of a solar cell in and outside a glovebox



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