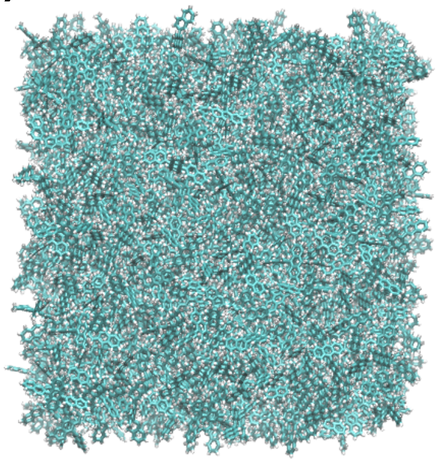
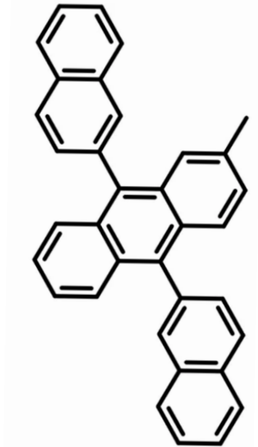
(a)



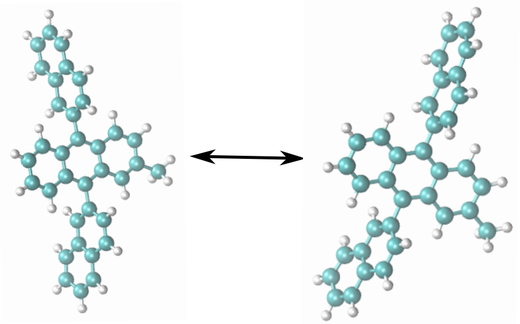
MD simulation of Morphology

(b)



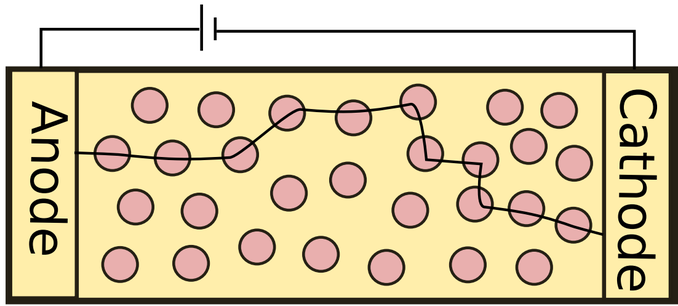
Molecule Energy Calculation: E_i

(c)



Reorganization energy and coupling element calculation: λ_{ij}, J_{ij}

(d)



Device dynamics simulation