Ground State Dimer Molecule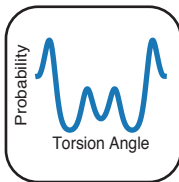 → Quantum Chemistry → Torsion Potential (Energy vs Torsion Angle) → Boltzmann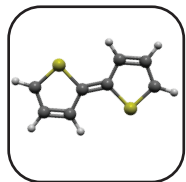 Distribution → Torsion Probability (Probability vs Torsion Angle) → Randomly Sample N_{GS} torsions → Single Chain Conformations
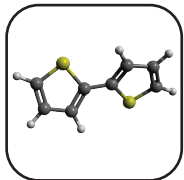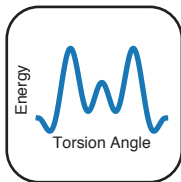
Doped or Excited Dimer Molecule → Quantum Chemistry → Torsion Potential (Energy vs Torsion Angle) → Boltzmann Distribution → Torsion Probability (Probability vs Torsion Angle) → Randomly Sample N_E torsions → Single Chain Conformations
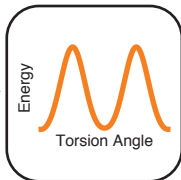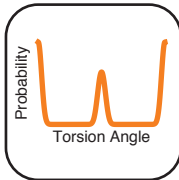
$$\alpha = \frac{N_E \text{ Torsions}}{N_{GS} \text{ Torsions} + N_E \text{ Torsions}}$$

N_{GS} torsion
N_E torsion

$\alpha = 0$
$\alpha = 0.5$
$\alpha = 1$