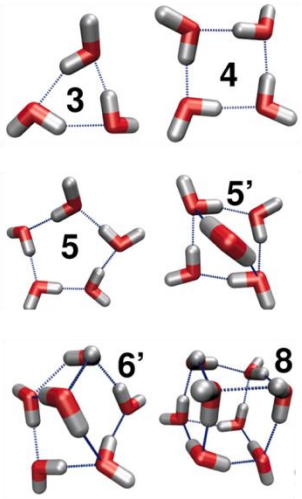
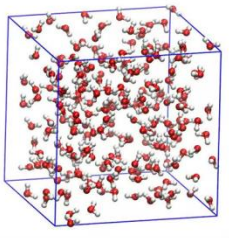
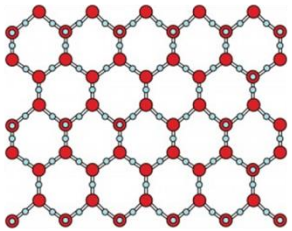
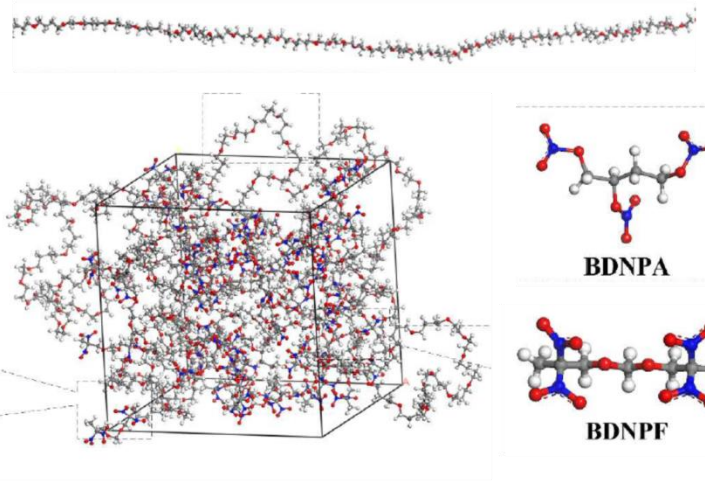
Multiscale Modeling Lab @ NTUST





Liquid





Molecule	Cluster	Solid	Polymer/Polymer blends
Space 1 Å		10~50 Å	10 nm
Time 1 fs		1 ~20ns	100 ns

Tzu-Jen Lin

Assistant Professor

Dept. of Materials Sci. & Eng.

Tel:+886-2-2737-6520

tjlin@mail.ntust.edu.tw

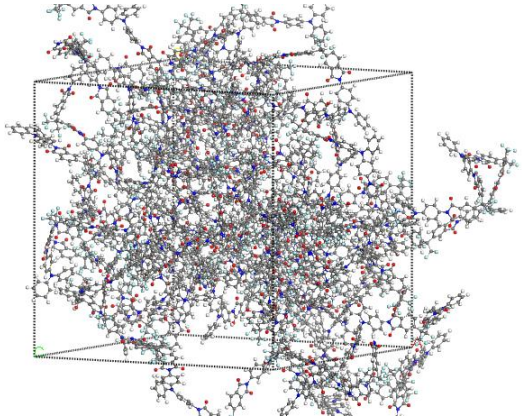
We are fascinated and engaged in studying physical chemistry problems from molecular level to 50 nanometer scale through quantum chemistry, first principle, and equilibrium/non-equilibrium molecular dynamics.

Multiscale Modeling Lab @ NTUST

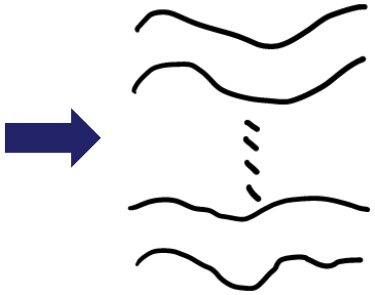
QSPR Modeling for Polymers

Polymer Chain Behavior ⟷ **Dielectric/Optical/Mechanical Prop.**

Molecular Dynamics Simulation ✚ Quantum Chemistry Calculation

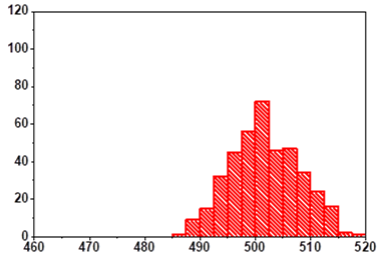


Bulk Polymer

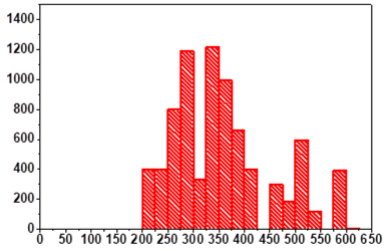


Polymer Chains

Polarizability



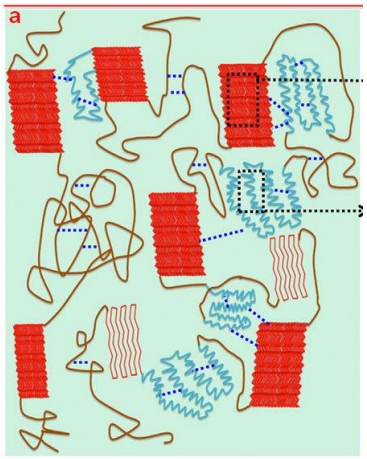
Rg^2



Analyzing Polymer Chains Data

Multiscale Modeling Lab @ NTUST

High thermal conductivity polymer



Materials	k [W m^{-1} K^{-1}]
NC dragline silk [a)]	349, 416
Silkworm silk ⊥ [b)]	0.37[27]
Silkworm silk ∥ [b)]	2.4~4.7
Human hair	
Unperfused tissues[28]	~0.5
Kevlar 49	~30
Copper	401

Adv. Mater. **2012**, *24*, 1482–1486

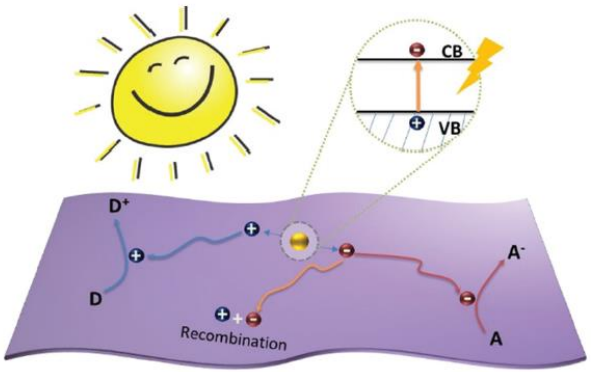
- No Free electrons
- Simple compositio
- No SP^2 in backbon

Multiscale Modeling Lab @ NTUST

2D Photocatalyst

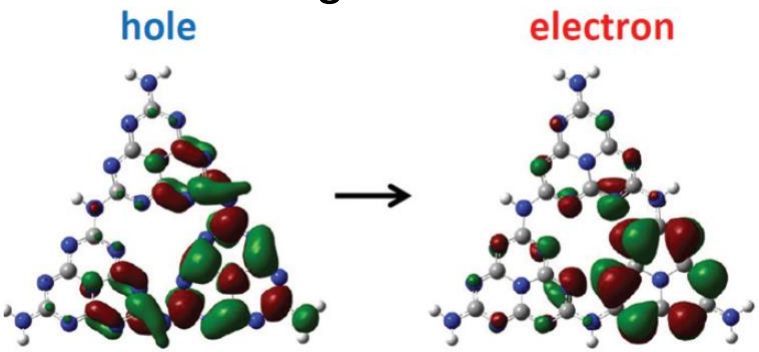
We are interested in how molecular structure, dopant, defect and heterojunction influence the optical and chemical property of 2D photocatalyst

Photocatalytic process

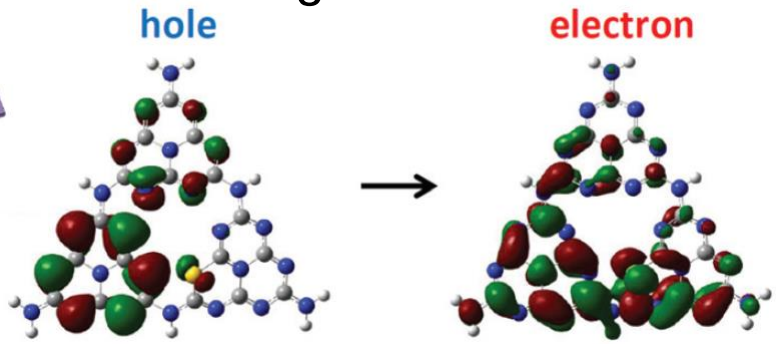


Nanoscale, 2016, 8, 6904-6920

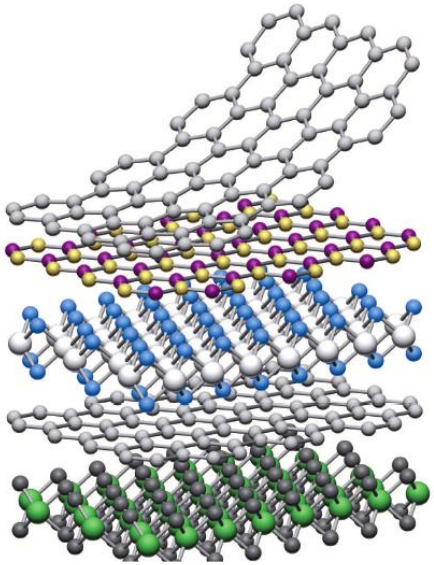
g-CN



g-CN-S

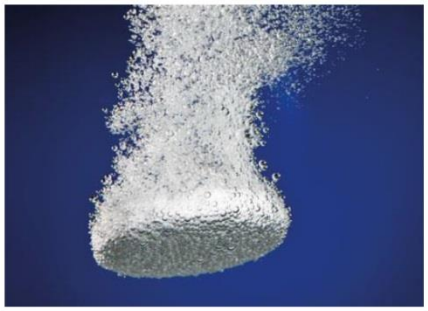


2D Heterojunction

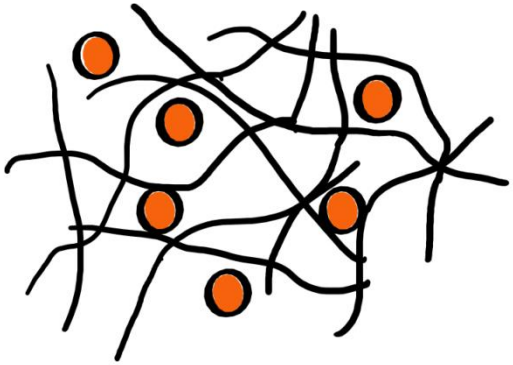


Multiscale Modeling Lab @ NTUST

Amorphous Solid Dispersion



Crystallization of drug molecules in polymer matrix diminish their aqueous solubility

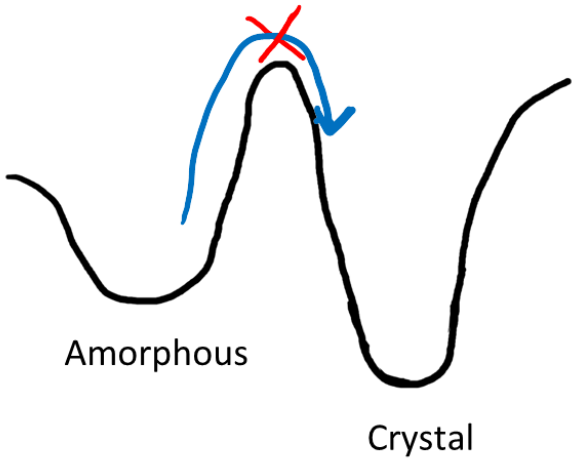


Drug Molecule Polymer

Simulation

- **Tg / Viscosity calculations**
- **MSD: Polymer Chain and Drug Molecule**
- **Chain conformation**

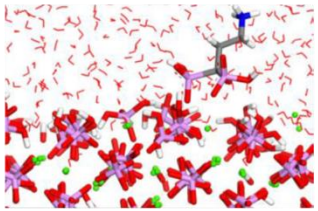
- **Would drug molecules recrystallize in amorphous polymer matrix?**
- **Molecular mobility is key**
- **Dry spraying experiments are time-consuming**



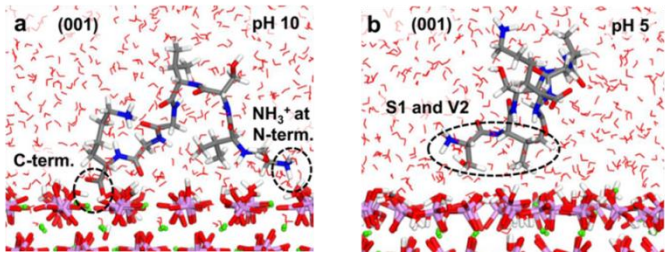
Multiscale Modeling Lab @ NTUST

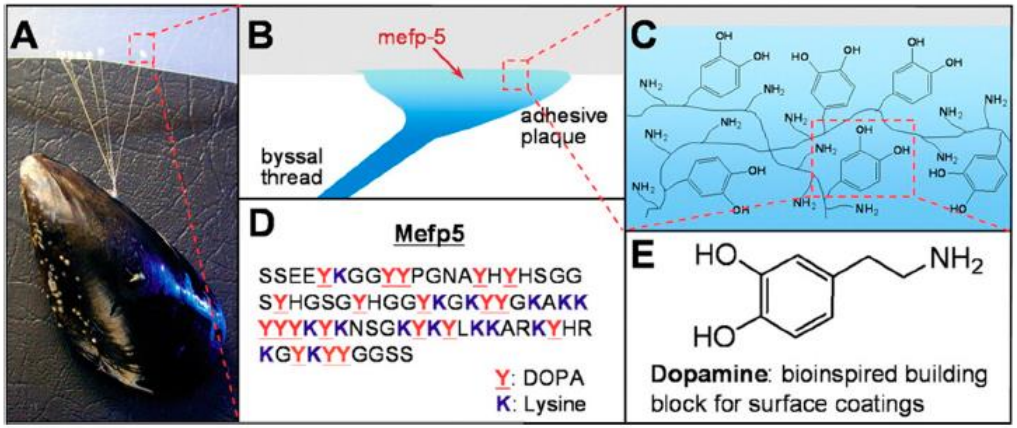
Polymer/Peptide adsorption on inorganic material (Au, Ag, Pt, Pd, Cu, SiO_2, Al_2O_3, HAP) surfaces

Bisphosphonate binding to HAP surfaces



SVSVGGK binding to HAP surfaces with different degrees of protonation





Science 2007 Oct 19;318(5 849):426-30. doi: 10.1126/science.1147241

Simulations in organic/inorganic interfaces provide useful information for designing adhesive materials in wet environment