HPC Meets Big Data

Manaschai Kunaseth

National Nanotechnology Center (NANOTEC)

National Science and Technology Development Agency (NSTDA)

Thailand Science Park, Pathum Thani, THAILAND

manaschai@nanotec.or.th

Biography

manaschai@nanotec.or.th

Manaschai Kunaseth

- Researcher
- Nanomaterials and Nanosystems Engineering Unit, NANOTEC

Research interests:

Computational chemistry:

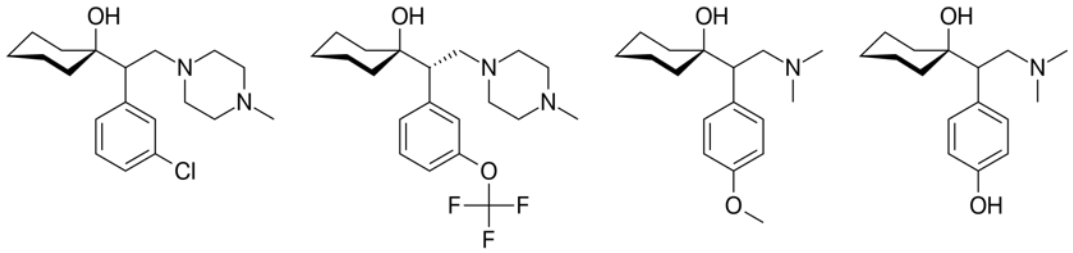
- DFT simulations: Catalytic chemical & reactions, adsorbent design
- Reactive MD: Method development

Computer Science:

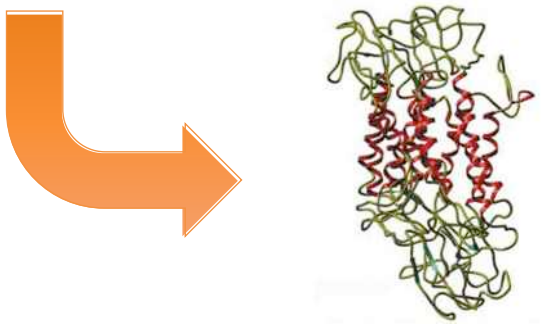
- Parallel algorithm design and analysis on massive-scale supercomputers
- Data analysis and visualization

HPC Meets Big Data: Computer-Aided Drug Design

- Finding key (drug) for the lock (target protein)



WY-46824 WAY-256805 venlafaxine desvenlafaxine



Anti-depressant drug:
Serotonin–norepinephrine reuptake inhibitor:
Cycloalkanol ethylamine scaffold

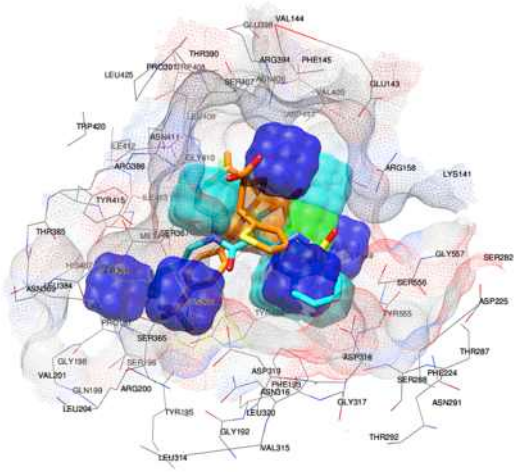
- Quantitative Structure-Activity Relationship (QSAR)

Predictor → **Activity**

- Experiment
- Simulation

Regression/
Classification
e.g. SVM, PLS

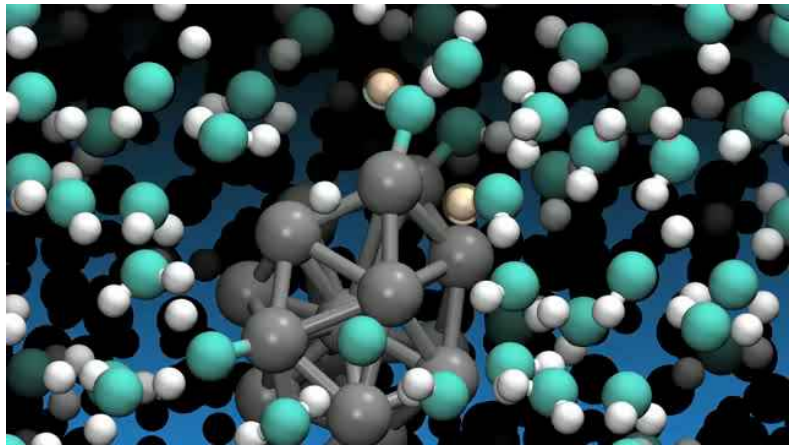
- Experiment
- Simulation



3D QSAR

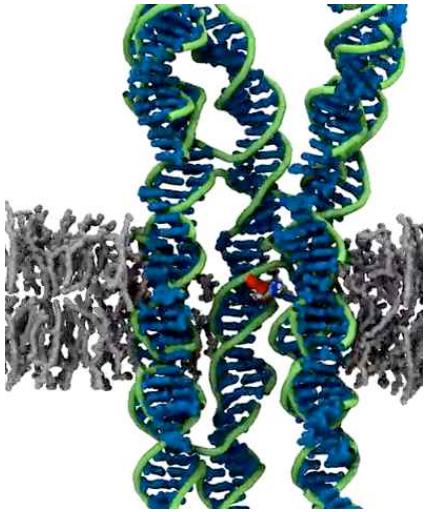
HPC Application: Molecular Simulation

- **QM: Density functional theory (DFT)**
  - Degree of freedom: *Electron density, atom positions*
  - A first-principle calculation
  - Computationally expensive (atoms < 500)



H_2 production from Al superatoms. (Adapted from Ohmura *et al., J. Chem. Phys.* (134(24):244702 (2011))

- **MM: Molecular dynamics (MD)**
  - Degree of freedom: *Atomic positions*
  - Empirical force-fields
  - Less expensive (atoms < 10^6-10^7)



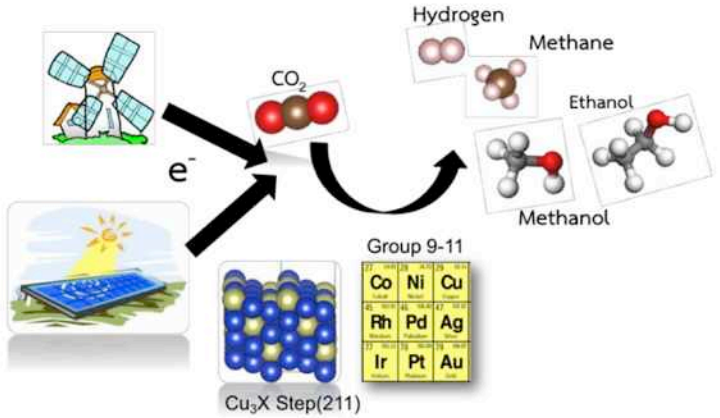
ATP molecule passes from one side of the membrane to the other through the transmembrane pore. (Adapted from Yoo & Aksimentiev, *J. Phys. Chem. Lett.* 6 4680-4687(2015))

Catalysis for Energy Production

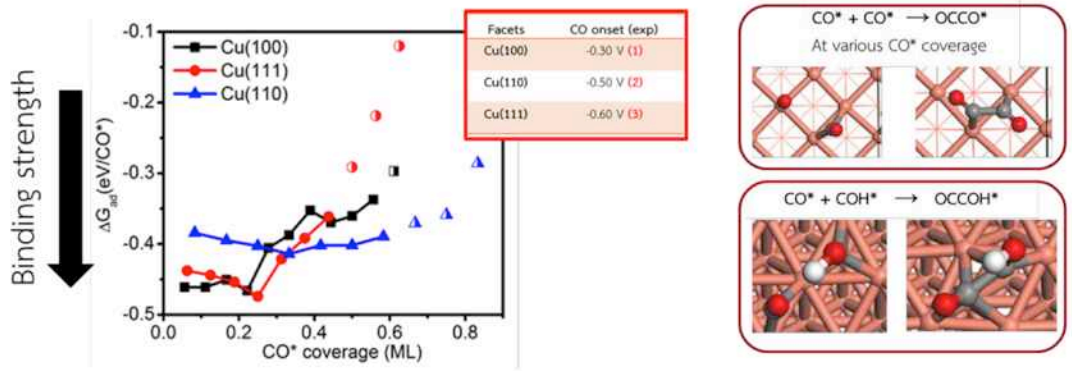
NANOTEC a member of NSTDA

CO_2 Electrochemical Reduction to Methanol and Methane on Stepped Cu-based Alloys (211) Surfaces

P. Hirunsit *et al. J. Phys. Chem. C* 2013, *117* (16), 8262-8268.
P. Hirunsit *et al. J. Phys. Chem. C* 2015, *119* (15), 8238-8249.

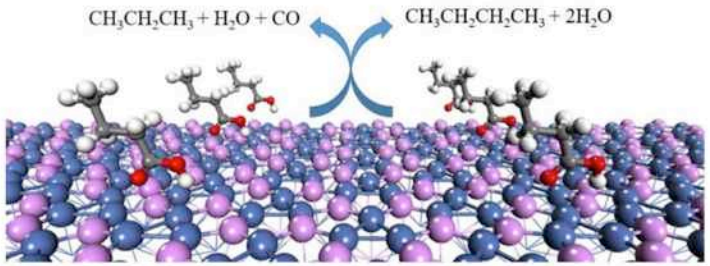


CO_2 Electrochemical Reduction to Ethylene on Cu(100), Cu(110) and Cu(111) Surfaces (Collaboration with Jason Yeo at NUS)

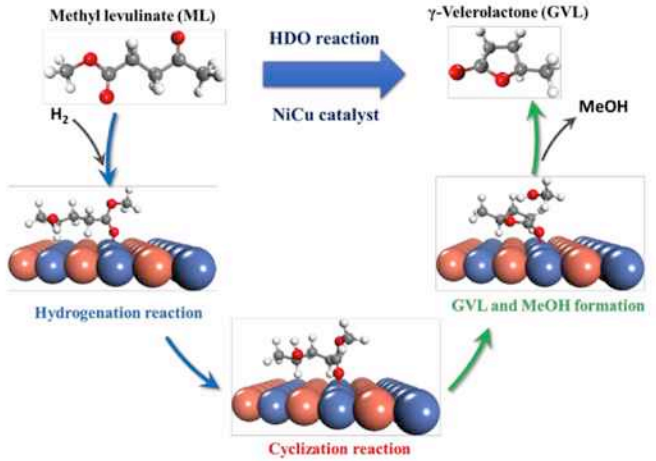


Y. Huang *et. al.*, *ACS Catal.* 2017, 7, 1749−1756.

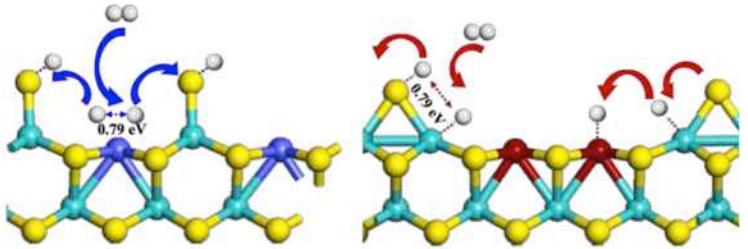
Palm Oil Conversion to Biofuel using Ni_2P Catalyst



Catalytic Transfer Hydrogenation for γ-Valerolactone (GVL) using NiCu Alloy



H_2 Activation on Partially Promoted Metal Edge of CoMoS and NiMoS



C. Sattayanon, *et al., Fuel Process. Technol.* 2017, 166, 217.

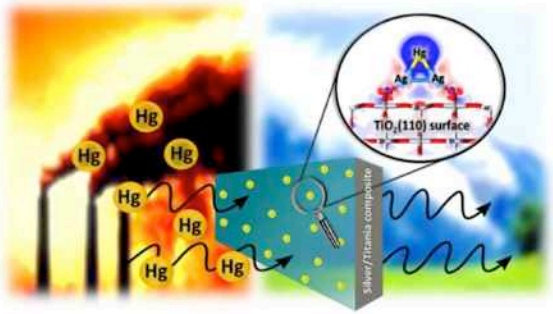
NSTDA

NANOTEC a member of NSTDA

Catalysts and Adsorbents for Pollutant Removal

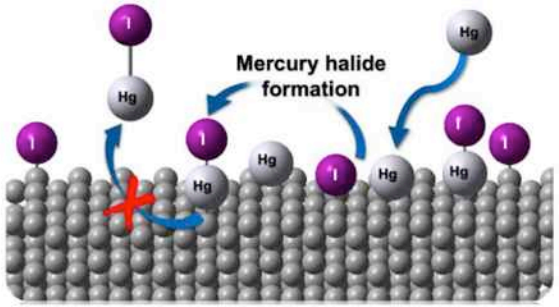
Development of Nanomaterials for Hg Removal

TiO_2-supported metal nanoparticles for Hg^0 removal



C. Rungnim, *et al., Chem. Eng. J.* 2015, 274, 132-142.

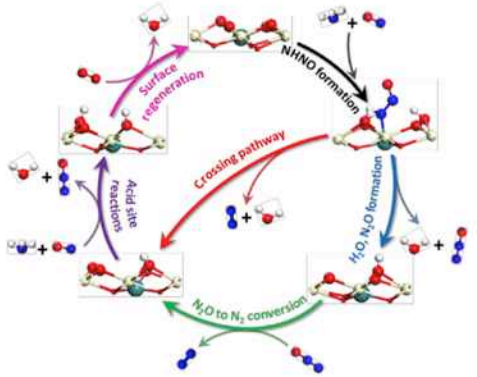
Activated carbon for Hg^0 removal



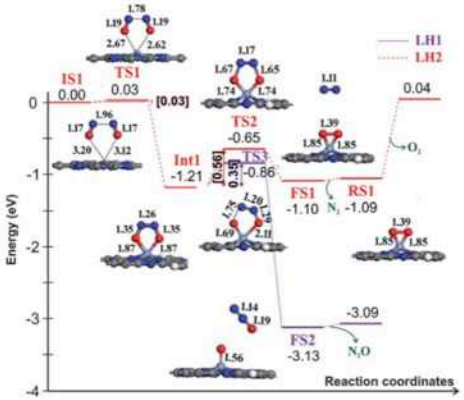
C. Rungnim *et al., J. Hazard. Mater.* 2016, 310, 253-260.

Nanomaterials for NO_x Removal

SCR-NH_3 of NO in metal oxide-based catalysts

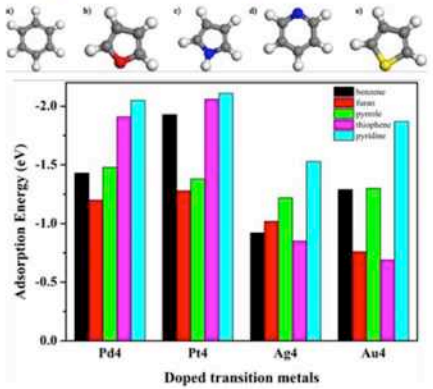


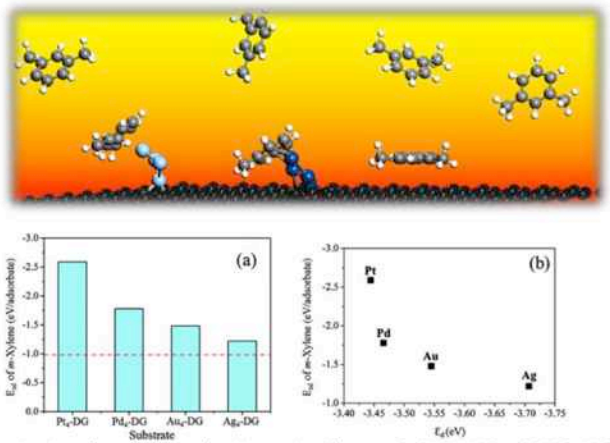
NO reactions in Metal complex and carbon-based catalysts



J. Meeprasert *et al., RSC Adv.* 2016, *6*, 20500-20506.
A. Junkaew *et al., RSC Adv.* 2017, *7*, 8858-8865.

Metal Deposited Defective Graphene for Volatile Organic Compound Removal

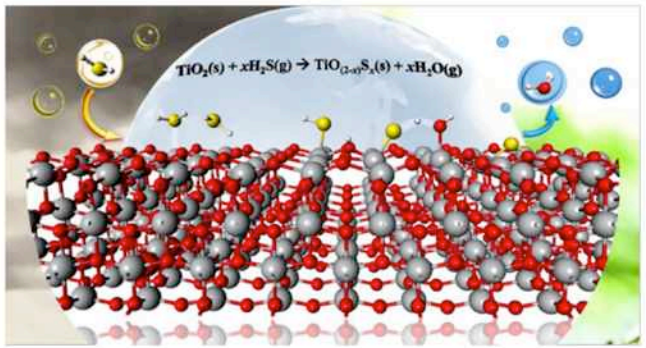




M. Kunaseth *et al. Appl. Surf. Sci.* 2017, 396, 1712-1718.

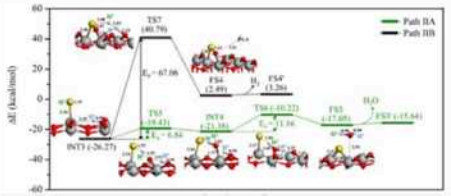
A. Junkaew *et al., New J. Chem.* 2015, 39, 9650-9658.

Nanomaterials for H_2S Desulfurization



$TiO_2 + xH_2S(g) \rightarrow TiO_{(2-x)}\text{-}S_x^* + xH_2O(g)$

$TiO_2 + xH_2S(g) \rightarrow TiO_2\text{-}S_x^* + xH_2(g)$



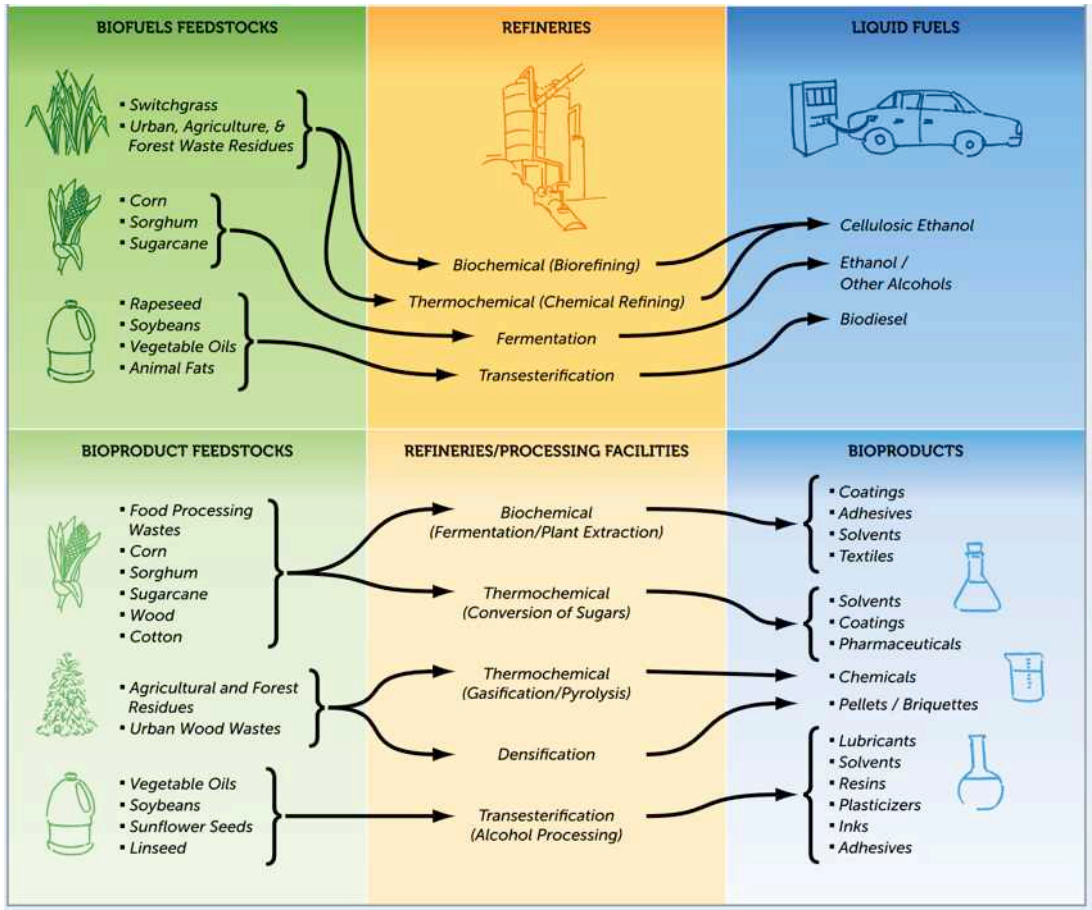
A. Junkaew *et al., Catal. Sci. Technol.* 2017, 7, 356-365.

Biorefinery

- **Biorefinery** integrates biomass conversion technologies to product biopower, biofuels, and bioproducts

- Biorefinery in Thailand's Strategic Plan:
  - Thailand's New S-Curve
  - NSTDA focused research (Bioeconomy)
  - Potential project in EECi (NANOTEC)
  - Integrated platform (bio-based material)

- Multi-national centers collaboration
  - MTEC, BIOTEC, NANOTEC



Source: United Stats Environmental Protection Agency and the National Renewable Energy Laboratory, State BioEnergy Primer, 2009

HPC & Big Data Applications: Similarities and Differences

- Both require huge computing power
  - HPC: high computation per byte (computation & memory-bandwidth bound)
  - Big Data: Low computation per byte (disk access & network transfer bound)

- Data point obtain from HPC application (and other scientific simulation) is usually expensive