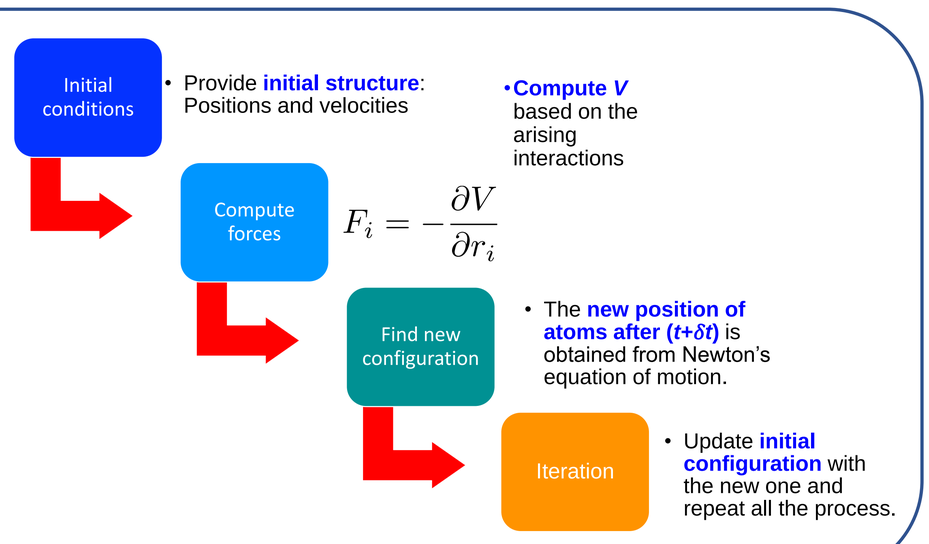
Sakti Laboratory

Department of Chemistry and Biochemistry, Waseda University

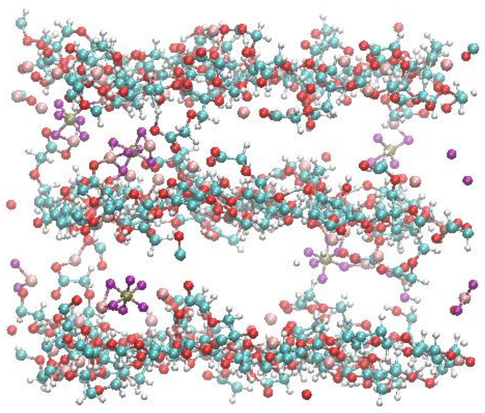
Computational Chemistry, Molecular Simulation

Sakti Laboratory is a Computational Chemistry lab that mainly uses molecular dynamics (MD) simulation. With MD simulation, we can investigate various molecular motions involving time and space by solving the equation of motion. Our research focuses on investigating chemical phenomenon using computational and theoretical approaches at both classical and quantum mechanical levels. We also develop new methods and models for designing new materials and molecules.



Batteries development

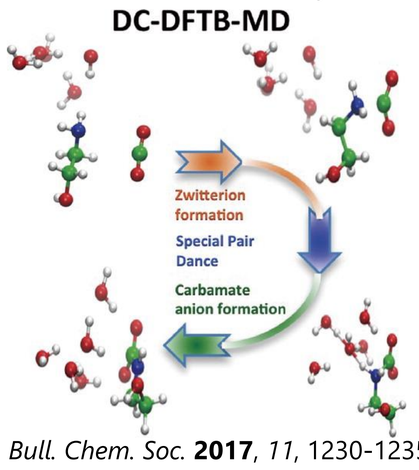
Due to the rapid development of electric devices, rechargeable batteries require high voltage capacity and energy density. We use MD simulations to simulate the behavior of ions in batteries.



We simulate the structures of a carboxymethyl cellulose electrolyte with ions. Cellulose electrolyte is an eco-friendly and safe solid-state electrolyte. Our goal is to find the best modified cellulose for use as an electrolyte without expending resources.

Carbon capture analysis

We are addressing environmental problems by developing materials that absorb CO_2 and convert it into fine chemicals. Reducing and utilizing CO_2 will contribute to a sustainable society.

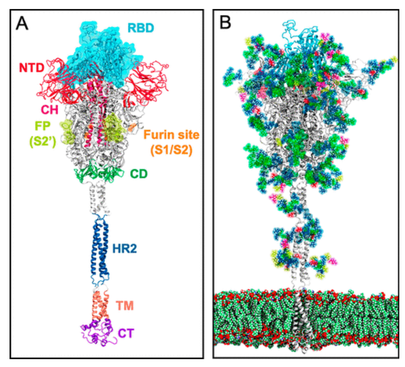


Bull. Chem. Soc. **2017**, *11*, 1230-1235.

We performed MD simulation to elucidate the process of CO_2 absorption, including the formation of carbamate anions and the diffusion of hydroxide ions.

Vaccine design/drug discovery

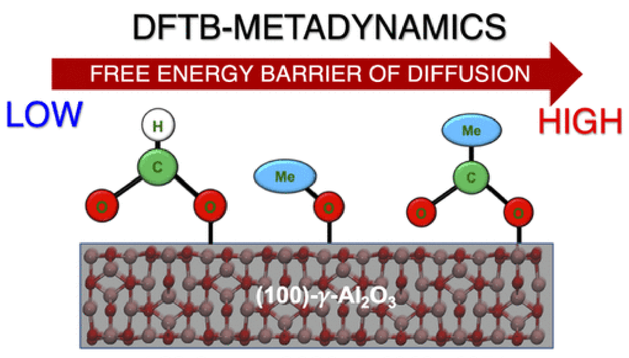
We can use machine learning, molecular docking, and MD simulations to investigate millions of candidate compounds for drugs simultaneously. This makes computational simulation an efficient way to find drugs and helps experimentalists choose initial targets.



MD simulation can investigate biomolecular motions and rapid reactions that are difficult to observe experimentally due to space and time limitations. We use simulation to elucidate mechanistic information about reactions involving biomolecules.

Catalytic reaction simulations

Catalysts are used in various aspects of our daily life. For example, three-way catalysts such as noble metals and metal oxides are used to eliminate hazardous exhaust gases (CO, NO_x, and unburnt C_xH_y).

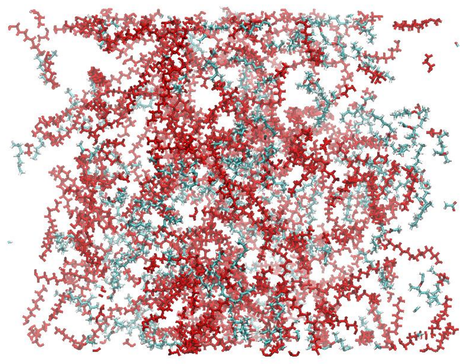


ACS Omega **2020**, *5*, 6862−6871.

MD simulation was performed to elucidate the diffusion process of several oxy-carbon species on catalytic surfaces. This diffusion process is significant for reaction efficiency.

Liquid phase simulations

Solutions can have various possible structures due to collisions or interactions among molecules. It is impossible for static calculations to consider all these structures, so MD simulation is a suitable way to investigate molecular motions in liquid systems. We use MD simulation to elucidate proton and hydroxide ion transfers in water.



Simulation for liquid systems can be applied to many models, such as carbon capture by amine solution and aqueous sodium-ion batteries.

Software development

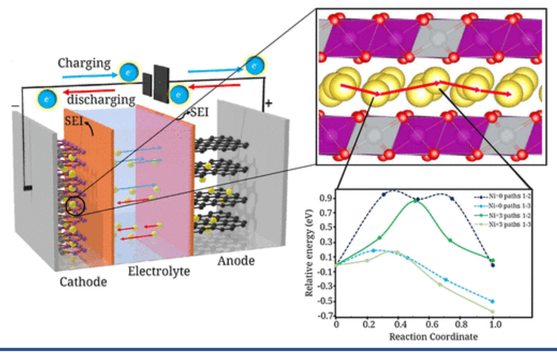
CMMDE is new platform for quantum and classical calculation. It is a set of Python scripts to setup, run, analyze, and visualize jobs in computational molecular and material design. With CMMDE, people can automatically execute various calculation methods. There is no need to make long complicated input files and scripts.

CMMDE

Removing the barriers in Computational Chemistry research

Researchers can use CMMDE to perform molecular simulations even if they are not familiar with the programs. This tool will contribute to the education and development of computational chemistry.

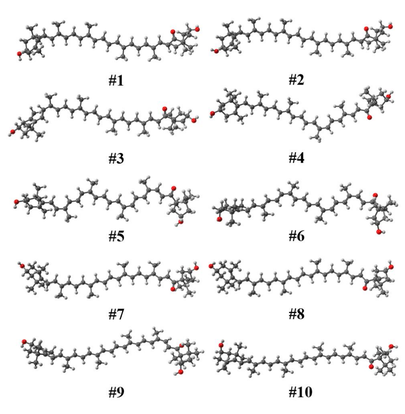
Recent Work



$Na_2Mn_{3-z}Ni_zO_7$ material for sodium-ion battery

Sodium is more abundant in nature compared to lithium. Moreover, sodium-ion batteries have a similar structure to lithium-ion batteries. We have performed MD simulations to elucidate the process of ion transfer in these batteries.

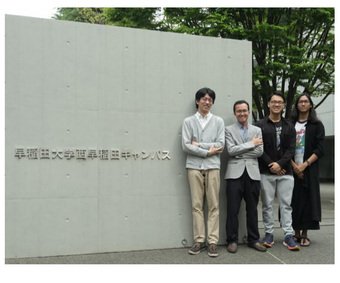
J. Phys. Chem. C **2022**, *126*, 20754–20761.



Quantum Chemical assessment on the optical properties of capsanthin

Capsanthin, as a natural dyes obtained from chilies, is a potential compound for photosensitizer in dyes-sensitized solar cells application (DSSC). The capsanthin molecule can have multiple conformers that exhibits different electronic and optical properties.

Under review in Journal of Computational Chemistry.



In 2023, Sakti Lab has two undergraduate students and one graduate student. We mainly use molecular simulation as a tool to unlock physical and chemical properties of various materials in a broad range of applications. We are welcoming any prospective students who are interested in playing with molecules and their motions in our lab.

Access HP

https://www.saktilab.org/