

Research theme: Elucidation of the paths and reaction rates of combustion chemical reactions


Name	FUSHIMI Ryota	E-mail	r.fushimi@hakodate-ct.ac.jp
-------------	---------------	---------------	-----------------------------

Status	Assistant professor
---------------	---------------------

Affiliations	Combustion Society of Japan
---------------------	-----------------------------

Keywords	Combustion chemistry, Chemical kinetics, Radical, Reaction rate coefficient
-----------------	---

Technical Support Skills	• Exploration of reaction using computational chemistry • Evaluation of the practical feasibility of new fuels
---------------------------------	---

Research Contents
Tracking of the initial oxidation reactions in combustion using quantum chemical calculations

As the establishment of a carbon-neutrality, or zero-emission society, highly efficient combustion methods and new fuels that do not rely on fossil fuels are needed. However, conventional developments based on trial-and-error are thought to be limited in terms of both cost and time. Therefore, successful social implementation requires understanding the specific chemical reactions and ignition processes that occur under various conditions.

It is known that the reactivity of intermediates formed during combustion reactions significantly influences the ignition of hydrocarbon-based fuels, which are currently the most widely used in transportation. While the reactivity of fuels lacking double bonds (alkanes) has been thoroughly investigated and understood, the reaction behavior of molecules containing double bonds (alkenes) remains to be elucidated.

This study focuses on the initial reaction products of alkenes and their reaction kinetics. Their reaction mechanisms are investigated using quantum chemical calculations at a level of detail that is beyond the reach of experimental observations.

Metal fuels have attracted considerable attention as carbon-free energy carriers because of their potential applications, particularly in space exploration and rocket propellants. Aluminum and magnesium are currently regarded as the most promising candidates among them. However, their combustion characteristics differ substantially from those of hydrocarbon fuels. Resolving these issues requires a detailed understanding of how small metal oxide clusters, consisting of only a few atoms, react and subsequently aggregate. Furthermore, different metals are expected to follow distinct reaction pathways, leaving many fundamental aspects of metal combustion unresolved.

This study focuses from the initial stage to the final stage of metal combustion, gas-phase reactions and particle aggregation and solidification, with particular emphasis on the growth of metal oxide clusters containing up to several tens of atoms. Quantum chemical calculations and molecular dynamics simulations are employed to elucidate the underlying reaction mechanisms.

Available Facilities and Equipment
