1

Introduction

Ji-Jun Zou

Tianjin University, Key Laboratory of Advanced Fuel and Chemical Propellant of the Ministry of Education, Key Laboratory for Green Chemical Technology of the Ministry of Education, Department of Chemical Technology, School of Chemical Engineering and Technology, 92 Weijin Road, Tianjin 300072, China

The aerospace technology has undergone tremendous development since the first flight by Wright Brothers in 1903, which has significantly improved the life quality of human being and extended the capability of space explosion. Nowadays the aerospace vehicles mainly include commercial/military airplanes, missiles, rockets, spaceships, and satellites, which equipped with turbine, turbofan, ramjet, or rocket engines. Most of them apply liquid fuels majorly including hydrocarbon-based and hydrazine-based fuels. Hydrocarbons are the sole liquid fuel of airplanes, most missiles, and some rockets, meanwhile hydrazine and its derivatives are solely used for rockets for space exploration. Hydrocarbons have obvious advantages of safety and nontoxicity compared with hydrazine; thus many rockets using hydrocarbons have been used.

The primary role of liquid fuels is to provide energy source for propulsion, so the energy density of fuels is critically important because to a large degree it can determine the flight distance and payload of vehicles. Of course, fuels with high-energy density are always desirable because they can provide sufficient energy to enhance the flight performance. With the same fuel tank, the utilization of high-energy density fuels can extend the flight distance, increase the payload, or increase the cruise endurance. Otherwise, the volume of fuel tank can be reduced when using high-energy density fuels; thus the more space is accessible for loading or the overall volume of vehicles can be greatly reduced. This is especially important for volume-limited vehicles like battle planes, unmanned aerial vehicles, tactical missiles, spaceships, and satellites, for which the space for fuels is strictly restricted.

Traditional liquid fuels produced from petroleum refinery industry, like widely used jet kerosene and rocket kerosene, possess relatively low energy density (<34 MJ/l). And high-energy density fuels generally have energy density higher than 36 MJ/l, which is a result of density multiplied by mass energy. To get high-energy density fuels, synthesis chemistry is the first choice, for which two ways can be used. One is to synthesize polycyclic and diamondoid hydrocarbons with

High-Energy-Density Fuels for Advanced Propulsion: Design and Synthesis, First Edition.
Edited by Ji-Jun Zou, Xiangwen Zhang, and Lun Pan.

contact cyclic structure to afford high density (called high-density fuels); however its mass energy is not increased or even slightly decreased due to the lowered H content. The other is to synthesize strained cyclic hydrocarbons, which not only provide high density but also increase the mass energy attributed to the additional trained energy in the molecules, and thus is more effective to increase the energy density. Actually, the synthesis chemistry of high-energy density fuels has been rapidly developed. However, it is difficult to further increase the energy density of hydrocarbons, so many new approaches have been explored, like the addition of energetic nanoparticles in hydrocarbons to get nanofluid and gelled fuels. Also, as response to the sustainable development, producing high-energy density fuels from renewable source like biomass has become a hot topic, which is different from the synthesis of common biojet fuels and requires more sophisticated synthesis. Moreover, the applications of high-energy density fuels have been extended from traditional vehicles to many advanced vehicles that often work under adverse circumstances. In this case how to realize the energy of fuels to maximum degree is a big challenge; for this purpose it is necessary to enhance the ignition and combustion of fuels. It is also worth noting that the reason for the wide use of toxic hydrazine derivates in rocket engines as fuel of bicomponent propellant is the excellent hypergolicity of hydrazine, which can ensure the reliability and avoid the use of complex ignition device. To replace toxic hydrazine derivates, it is necessary to develop safe and green hypergolic fuels. And energetic ionic liquids have been proved as a good choice, although its energy density is not so high.

Besides the high-energy density, advanced fuels must satisfy several specifications for application, such as low-temperature fluidity, thermal oxidative stability, combustion characteristics, compatibility with materials, and volatility. The structure and composition of fuel must be finely controlled, which depends on the synthesis technology that may include several aspects of synthesis chemistry such as design of fuel molecules, design of synthesis route, understanding of reaction mechanism, design and fabrication of catalyst, integration and scale-up of reaction, etc.

This book will cover the theory and practice of designing, synthesizing, and improving the performance of fuels and connect the road from the past, current, and future of fuel chemistry and technology. In the following Chapters 2–9, we will comprehensively and systematically demonstrate the concept, design, and synthesis of high-energy density fuels and its potential in improving the performance of aerospace vehicles. The contents range from polycyoalkane fuels, strained fuels, alky-diamondoid fuels, and hypergolic and nanofluid fuels derived from fossil and biomass (Figure 1.1), including molecular design, synthesis route, physiochemical properties, and their application. Chapter 2 will summarize the development history and basics of aerospace fuels including traditional fuels and high-energy density fuels. Chapter 3 will present the design and synthesis of high-density polycyoalkane fuels, with the catalyst and reaction optimization as focus. Chapter 4 will introduce the synthesis of high-density diamondoid fuels and focus on two control synthesis routes. Chapter 5 will introduce the design and synthesis of high-energy strained fuels, in which the synthesis will extend from liquid to solid strained hydrocarbons. Chapter 6 will summarize the design

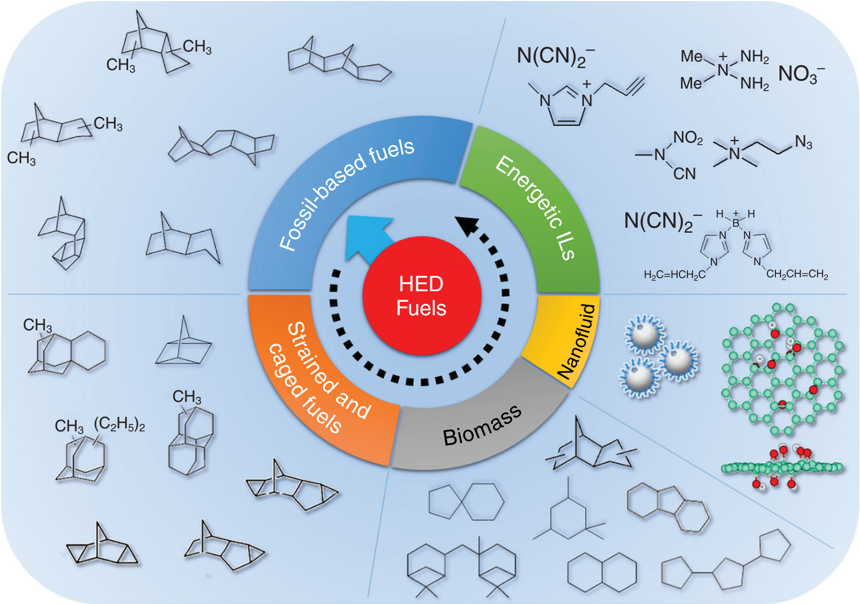

Figure 1.1 The synthesis and upgrade of high-energy-density fuels including fossil, biomass, nanofluid, and ionic liquid-based fuels for aerospace propulsion. Source: Zhang et al. (2018). Reproduced with permission of Elsevier.

and synthesis of high-density fuels from biomass derivates, including the typical reaction route, catalysts, and mechanism. Chapter 7 will show synthesis of energetic nanofluid fuels and the gelling technology to stabilize them. Chapter 8 will present the design and synthesis of green hypergolic liquid fuels and show it potential to replace toxic hydrazine. Chapter 9 will focus on how to improve the combustion properties of high-energy density fuels.

Reference

Zhang, X.W., Pan, L., Wang, L. et al. (2018). Review on synthesis and properties of high-energy-density liquid fuels: hydrocarbons, nanofluids and energetic ionic liquids. *Chemical Engineering Science* 180 (28): 95–125.