Electronic structure of strained hydrocarbons as liquid high energy density (HED) aerospace fuels

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Liquid hydrocarbons (HCs) have been the major energy source for aerospace technology although the Apollo Mission used liquid hydrogen as fuel over 50 years ago. The energy density of fuels is critically important because it determines the flight range and payload of aircrafts [1]. High-energy-density (HED) fuels have been developed with considerable progress in the past 20 years in aerospace technology. The energy density of fuel is directly determined by the density and volumetric net heat of combustion (NHOC), which is linearly correlated to HED of the fuels. As a result, liquid fuels with both high energy (HE) and HED are required for the volume and weight-limited aircraft.

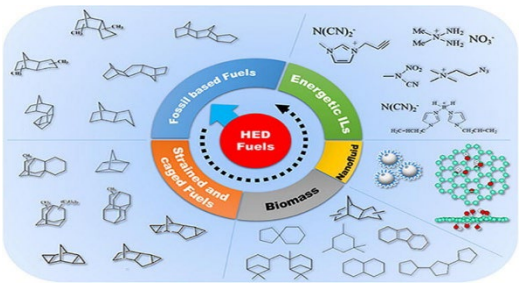

Fig 1 strained hydrocarbons and their applications [2].

It is discovered that some stained multi-cyclic HCs as shown in Figure 1 [2] with pentagon or hexagon rings of provide more combustion heat. It further discovers that the multi-cyclic HCs with relatively low H/C ratio (high molecule weight) and more highly strained rings will show both HE and HED properties [1]. For example, the strained quadricyclane (QC) shows 18% higher density than the Rocket Propellant-1 (RP-1) and or PR-2 fuels which are highly refined form of kerosene, used as rocket fuel. Properties of HED fuels are directly determined by their molecule structures. As a result, understanding of these strained HCs as energy materials in order to design and develop new type of advanced fuels. In the present study. In this presentation, I will discus our recent study in strained HCs in particular electronic structure and spectroscopy [3-4] of strained HCs and their design in aerospace fuels.

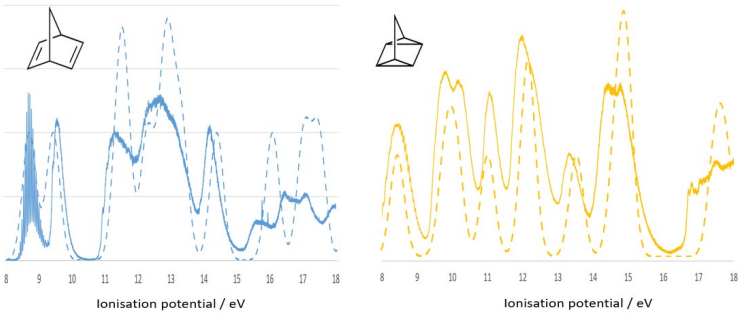

Fig 2 Comparison of calculated ionization energy spectra of NBD and QC with recent synchrotron sourced PES [2].

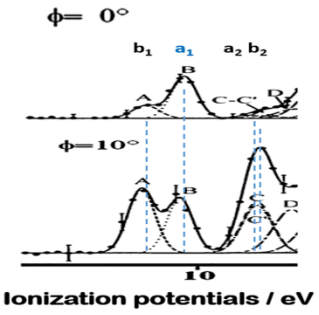

Fig 3 Outer valence spectra of NBD using EMS [4].

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