energy density, a nd the

potential to be employed in e xisting transportation infrastructure where fossi l fuels currently dominate. While i t has many

beneficial properties, a hydrogen-based fuel is challenging to synthesize due to the chemical properties of elemental

hydrogen. Hydrogen al one is not an effective fuel, nor does it readily re act wi th ot her molecules required for its

conversion to a liquid form with superior fuel properties. Therefore, a catalyst is required to facilitate the chemical

react ions required for producing a practic al hydrogen-based fuel. The complete process, from the production of our

proposed hydrogen-based fuel to its combustion in transportation vehicles, is a fully renewable and carbon-neutral

process.

Molecular hydrogen (H2) can be obtained from the electrolysis of water (H2O)

using renewable e nergy such as wind or solar power. To be converted to a practical fuel,

hydrogen must be chemically combined with a carbon source such as carbon dioxide

(CO2). My research focused on a novel method of catalyzing these reactions, which

leverages the principles of Hard-Soft Acid-Base (HSAB) theory. According to HSAB

t heory, hard aci ds tend to form strong bonds t o hard ba ses, while soft acids prefer to

bond to soft bases. We hypothesized that a proposed chemical cata lyst such as Si lver

Fluoride(AgF), whi ch contains a mismatche d soft acid and hard base, could split

m olecular hydrogen into two se parate hydrogen ions capable of bonding

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the reaction, we needed to attach a N-Heterocyclic Carbene

l igand (NHC ligand) to AgF. NHC ligands are large mole cules that improve t he bonding

and reactivity properties of metal molecules such as AgF.

Most of my t ime this summer was spent synthesizing a specific NHC ligand called IPr**. This ligand was

previously proven to improve the reactivity of

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i n our IPr** product. Much of my time

w᥵熆塑戰䖒İ楦Ⅶ㑈ቐ퀄怀 y summer research experi ence. I’m very

grateful for the opportunity to engage in Professor Tate’s Synthetic Chemistry laboratory and expand my chemistry

knowledge.

Facul ty Mentor: Dr. Brandon Tate

Funded by the Kufe Family Researc h Fellowship

References:

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