Probing mechanisms and theory, from molecular interactions to process design, Jackson group efforts range from fundamental…:

- Novel aspects of hydrogen bonding, including hydridic-to-protonic
- Computational modeling to design and interpret reaction mechanisms and structures

…to eminently practical chemistry:

- “Green” catalysts and pathways from renewables to useful “petro-” chemicals
- Alkali metal reductants “tamed” by dispersion in silica or alumina

More information can be found at www2.chemistry.msu.edu/faculty/jackson/; two active areas are outlined below, where the common thread is mechanistic. By understanding molecular interactions and reactions we seek rules to design materials and processes with targeted characteristics. From the post-doc to the high-school level, scientists trained in the group have gone on to excellent positions in academia, industry, or governmental research.

**Hydridic-to-protonic hydrogen bonding:** Our discovery and studies of this interaction, AKA dihydrogen bonding, began with a high school student studying NaBH₄·2H₂O (Fig. 1). Besides the novelty of hydrogen’s serving as the nucleophile in a hydrogen bond, this work has uncovered reactions governed by the material’s phase and local stoichiometry as well as a bonfire crystal-to-crystal solid state transformation. Dihydrogen bonding projects have focused on crystal engineering; design of bond-selective infrared activated reactions; and searches for possible biological and synthesis significance.

**Green Chemistry:** We seek to replace fossil petroleum with renewables as the basis for chemicals and fuels via catalytic paths starting from biomass-derived feedstocks. Target products are commodity and specialty chemicals and fuels. Reaction optimization is guided by mechanistic explorations of rates, substituent effects, isotopic labeling, and variations in media and conditions. Meanwhile, new catalysts and reagents are also under development.

**Synergy:** Our catalytic and electrocatalytic reductions of bio-derived feedstocks in water (practical) now intersect with the dihydrogen bond (fundamental) work; interfacial dihydrogen bonding of metal-bound hydride sites under water seems to strongly affect their reactivity. In turn, the quest for “biomass refinery operations” via electrocatalytic reduction of bio-based feedstocks unexpectedly found aryl ether cleavage over a simple Nickel electrode (Figure 2). Such serendipities and synergies between practical and fundamental; synthesis, structure and mechanism; and experiment and theory pull us back to the lab each day.

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**Selected Publications**