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

- Nature, scope, and applications of hydridic-to-protonic hydrogen bonding
- Complexant design and synthesis for thermally robust alkalides and electrides
- Approaches to organic-based magnetic materials by self-assembly

...to eminently practical...

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

More information can be found at http://www.cem.msu.edu/~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 academics, 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).

Fig. 1. ORTEP images of the (unpublished) neutron diffraction structure of NaBD₄•2D₂O. These orthogonal views show the close D–D contacts between three D₂O molecules and one of the deuterons of the BD₄⁺ ion.

Besides the novelty of hydrogen’s serving as a nucleophile in a hydrogen 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 lactic acid unexpectedly found lactaldehyde in route to propylene glycol (Figure 2).

**Green Chemistry:**

With Prof. Dennis Miller (MSU Chemical Engineering), we aim to replace fossil petroleum with renewables as the basis for chemicals and fuels. Our catalytic paths upgrade bio-based feedstocks (e.g. carbohydrates, organic acids) to commodity and specialty building blocks (1,2-propanediol, chiral amino alcohols). Mechanistic insight—basic science—is key to process design—practical engineering—so we focus on adsorption, surface spectroscopy, and kinetic and quantum chemical modeling studies, complemented by classical mechanistic explorations of substituent effects, isotopic labeling, and variations in catalysts and conditions.

**Synergy:** Our studies of catalytic reductions of aqueous organic acids to alcohols (practical)

**Fig. 2. Electrocatalytic hydrogenation (ECH) of lactic acid over Ru/C particles at 70 °C converts the –COOH to –CHO. Reduction to –CH₂OH, the only product seen from “normal” hydrogenation, takes longer.**

are now intersecting 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 lactic acid unexpectedly found lactaldehyde in route to propylene glycol (Figure 2).

Our efforts now include crude biomass upgrading and catalytic reduction of cellulose, hemicellulose, and lignin to alcohols, olefins, and aromatics. In turn, the quest for "biomass refinery operations" via electrocatalytic reduction of lactic acid unexpectedly found lactaldehyde in route to propylene glycol (Figure 2).

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Besides the novelty of hydrogen’s serving as a nucleophile in a hydrogen bond, this work has uncovered reactions governed by the material’s phase and local stoichiometry as well as a bona fide crystal-to-crystal solid state transformation. Ongoing dihydrogen bonding projects focus on crystal engineering; a search for possible biological significance; and use of dihydrogen bonded systems as candidates for IR-pumped bond-selective vibrationally activated reactions.