

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

- Hydrogen bond insights, including hydridic-to-protonic and aromaticity-modulated systems¹⁻³
- Computational modeling to design and interpret reaction mechanisms and structures⁴⁻⁶

...to eminently practical chemistry:

- “Green” catalysts and pathways from renewables to useful “petro-” chemicals⁷⁻¹⁰
- Studies of bio-relevant solvents to connect molecular interactions to engineering properties.¹¹

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 academics, industry, or governmental research.

Novel Hydrogen Bonds: Our discovery and studies of hydridic-to-protonic H-bonding, AKA dihydrogen bonding, began with a HS student studying $\text{NaBH}_4 \cdot 2\text{H}_2\text{O}$ (Fig. 1a) and includes crystal engineering, searches for bio- and synthesis relevance, and infrared-activated bond-selective reactions.¹ We have also uncovered aromaticity/antiaromaticity-modulation of common H-bond strengths (AMHB, Fig. 1b) and have begun collaborative studies with chemical engineers to use our molecular-level understanding of H-bonding to develop practical models for properties and separations of alcohols and other bio-relevant liquids.²⁻³

Green Chemistry: We seek to replace fossil petroleum with renewables to make chemicals and fuels via catalytic paths starting from biomass feedstocks.⁷⁻⁹ Finite renewable carbon supplies call for C-retentive upgrading (i.e. reduction) of low-value lignin with energy from non-fossil sources. All these (wind, solar, hydro, nuclear) make electric power, so upgrading via electrocatalytic hydrogenation (ECH) is a focus, and has also turned up some novel ether cleavage and C-H activations (Fig. 1c). Having also uncovered very mild electrocatalytic C-H activation chemistry at HOC-H and $\text{R}_2\text{NC-H}$ sites in various molecules, we have now demonstrated that this activation process can be harnessed to use alcohols to alkylate amines, forming water

as byproduct (Fig. 1d). Meanwhile, mechanistic studies aid in design/optimization of catalysts and conditions.⁷⁻¹⁰

Synergy: Our catalytic and electrocatalytic reductions of bio-derived feedstocks in water (practical) and our C-H activation/amination chemistry now intersect with the dihydrogen bond (fundamental) work; interfacial dihydrogen bonding of metal-bound hydride sites under water may tune their reactivity. In turn, our AMHB studies (fundamental) are helping to inform the engineering solvent work (practical).¹¹ Such synergies between practical and fundamental; synthesis, structure and mechanism; and experiment and theory pull us back to the lab each day. 🌱

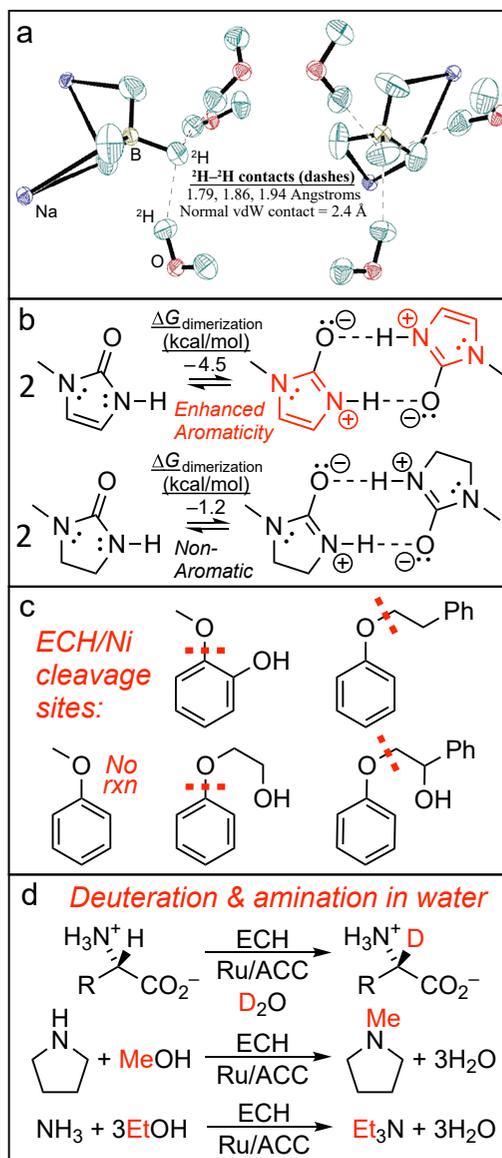


Figure 1. (a) Structure of $\text{NaBD}_4 \cdot 2\text{D}_2\text{O}$ showing close D...D contacts of three D_2O molecules to one BD_4^- deuteron; (b) Aromaticity-enhanced H-bonds vs. localized reference; (c) Surprisingly diverse ether bond cleavages promoted by mild (60 °C, aqueous electrolyte, skeletal Ni cathode) electrocatalytic reduction; (d) Mild aqueous electrocatalytic C-H activation and halide-free amination using simple alcohols.



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Mechanism and Design in Green and Organic Materials Chemistry

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