

# **The different facets of ice have different hydrophilicities:**

## **Friction at water / ice-I<sub>h</sub> interfaces**

Patrick B. Louden<sup>1</sup> and J. Daniel Gezelter<sup>1</sup>

<sup>1</sup>*Department of Chemistry and Biochemistry,  
University of Notre Dame, Notre Dame, IN 46556*

### **Abstract**

We present evidence that the prismatic and secondary prism facets of ice-I<sub>h</sub> crystals possess structural features that can reduce the effective hydrophilicity of the ice/water interface. This is shown through molecular dynamics simulations of solid-liquid friction, where the prismatic  $\{10\bar{1}0\}$ , secondary prism  $\{11\bar{2}0\}$ , basal  $\{0001\}$ , and pyramidal  $\{20\bar{2}1\}$  facets are drawn through liquid water. We find that the two prismatic facets exhibit roughly half the solid-liquid friction of the basal and pyramidal facets, and compare this difference to an idealized surface with tunable hydrophilicity. These simulations provide evidence that the two prismatic faces have a significantly smaller effective surface area in contact with the liquid water. The ice / water interfacial widths for all four crystal facets are similar (using both structural and dynamic measures), and were found to be independent of the shear rate. Additionally, decomposition of orientational time correlation functions show position-dependence for the short- and longer-time decay components close to the interface.