Someday the world’s liquid fuels needed for ships and airplanes will come from sustainable sources and low-energy processing. We are far from that day. While that fact is unfortunate, it opens up exciting opportunities for researchers from many different fields to work together to realize that vision. I will report on some of my research group’s contributions toward this goal, as we develop and apply quantum mechanics based simulation methods to unravel mechanisms associated with (photo)electrochemical water oxidation and carbon dioxide reduction at semiconductor electrodes and plasmon-catalyzed bond breaking over metal nanoparticles. The talk will focus primarily on CO$_2$ photoelectroreduction to fuel precursors but, time permitting, will also outline the potential for plasmonic catalysis to replace, e.g., the energy-intensive Haber-Bosch process. This latter work illustrates the potential to develop a non-thermal, low-pressure, visible-light-based approach to ammonia synthesis and hence to sustainable fertilizer production.