Recent years have seen huge advances in the accuracy and realism of first principles simulations. It is now an exciting time that issues such the role of van der Waals dispersion forces, quantum nuclear effects, and thermal (dynamical) effects can all be explored with first principles approaches. In this talk some of our work in this area will be discussed. This includes a consideration of the importance of quantum nuclear effects in chemical reactions at surfaces and in hydrogen bonding. I will also discuss how the friction of water at surfaces can be computed from first principles; revealing surprising results for the behavior of water at the surfaces of layered materials.