Molecular Dynamics at Metal Surfaces

Our recent work has focused on 1.) how to generate the correct electronic structure description for molecules at metal surfaces and 2.) how to propagate the dynamics of such molecules so as to properly allow for electron transfer and bond making/breaking (i.e. electrochemical dynamics). We will highlight here reasonably inexpensive strategies for accomplishing both tasks, including 1.) how to incorporate DMET (density matrix embedding theory) for treating impurity problems and 2.) a generalized surface hopping approach for treating open quantum systems. We will also discuss how these concepts can be applied and transformed so as to model realistic systems with ab initio potential energy surfaces (which is work that is going on right now).