

Building the World's greatest Microscope

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To observe, understand, and through this understanding, control the atomic scale motion involved in physical and chemical energy conversion processes is the central mission of SFB 1073. One might say it is our task to build and use the world's greatest microscope, a microscope that not only delivers still images but high speed movies fast enough to resolve atomic motion and in high enough resolution to see individual atoms. In this talk I will describe progress toward an unexpected type of "microscope": Atomically accurate dynamical simulations based on the first principles of Physics. I will show how molecular interactions at surfaces provide a test-bed for the development of this "microscope". In the course of this development, we discover that energy conversion can occur via unlikely mechanisms, where the adiabatic approximation separating the time scales of electronic and nuclear motion is found to be invalid. These insights suggest means for atomic scale control of energy conversion between reacting molecules present in the gas or liquid phase and solid state materials. Just as the collisions of molecules at the surfaces of solids represent two colliding worlds; this research direction represents an exciting interface for interactions between solid state physics and molecular science.