Modeling advanced materials with applications in solar energy conversion, chemical sensing, photocatalysis, and other fields is the focus of research in the Levine group. We apply the methods of computational chemistry to develop an understanding of the microscopic motions of nuclei and electrons in materials, and demonstrate how these motions determine the materials’ macroscopic properties. Students in my group will carefully apply a combination of quantum chemical and molecular dynamics techniques, developing and extending theoretical methods as dictated by the problem.

One goal of our research is to understand the properties of thin film and nanoscale semiconductor materials, which compose next generation solar cells and chemical sensors, are affected by the characters of their surfaces. These materials have desirable and tunable properties, and offer an inexpensive alternative to more traditional materials for solar energy conversion. Unfortunately, the non-radiative decay of electronic excitations at surface sites results in the conversion of electronic energy to useless heat, thus decreasing the efficiency of energy conversion. By constructing computer models of small clusters designed to mimic semiconductor surfaces, we inform the design of future materials by identifying the microscopic dynamics of such non-radiative decay.

In order to produce knowledge which most significantly impacts the development of next generation optoelectronic devices, we wish to extend the length- and timescales accessible via simulation. To this end, we take advantage of the similarity between the physical simulations and computer games by employing processors designed for gaming to accelerate our scientific computations. Through the development of algorithms and software, we work to take accurate first principles methods typically limited to the simulation of small molecules and extend them to the nanoscale.

The simulation of photodynamics requires the determination of ground and excited electronic wavefunctions at thousands of nuclear geometries. It is therefore necessary to use methods which are capable of quickly and stably calculating the electronic wavefunction of states of various characters (e.g. localized trap states vs. delocalized exciton states vs. charge transfer states). Multireference (MR) electronic structure methods provide such flexibility. With the above goals in mind, we are developing MR methods with lower computational cost, greater numerical stability, and greater accuracy than more widely used approaches for application in the study of semiconductor photochemistry.

In addition to modeling physical behaviors which cannot be directly observed, recent advances in computation and high performance computers allow researchers to approximate the results of experiments, thus saving time and effort. For example, much effort is spent experimentally screening molecules for various optoelectronic applications. Taking advantage of developments which allow the fast prediction of the photophysical properties of molecules in conjunction with genetic algorithms, we computationally evolve molecules with a desirable set of properties. By building trial molecules from a “primordial soup” of molecular fragments, testing their “fitness” for a given application using electronic structure methods, and automatically “mutating” and “crossing” them to produce fitter and fitter generations, we can search a massive molecular space for promising candidates before a single wet experiment is run. We hope this strategy will accelerate the development of materials for energy conversion, light emission, and other applications.

**Selected Publications**