

Theoretical and Computational Chemistry (Prof. Shih-I Chu)

General Research Focus:

The general research directions of Professor Chu's group are to develop new theoretical formalisms and *accurate* and efficient large-scale computational methods for in-depth *ab initio* investigation of chemical, physical, and astronomical processes of current significance in science and/or technology.

Recent Research Interests [<http://wavelet.chem.ku.edu/sichu>]

- Atomic and Molecular Physics in Strong Fields: Development of *non-perturbative* theoretical framework and both time-independent and time-dependent computational methods for accurate treatment of very-high-order (100th-300th order) multi-photon and nonlinear optical processes in intense and ultrashort laser pulses.
- Pioneering the development of *generalized Floquet formalisms* and *complex quasi-energy methods* for *non-perturbative* treatments of atomic, molecular, and optical (AMO) processes in intense *periodic* and *quasi-periodic* (multi-color) time-dependent laser fields.
- Development of *time-dependent generalized pseudospectral methods* for high-precision solution of time-dependent Schrödinger, Dirac, and Kohn-Sham equations in space and time.
- Development of *self-interaction-free* time-dependent density functional theory (TDDFT) for probing the *excited-state* electronic structure and dynamics of *many-electron* quantum systems (*atoms, molecules, clusters, quantum dots, nano-material,...*) with or without external fields.
- Quantum computing and quantum information.
- Attosecond (10⁻¹⁸ sec) technology and ultrafast science.
- Coherent and optimal control of microscopic quantum dynamics.

Most of these projects will require some background in physics, mathematics, computer program, and knowledge in classical and quantum mechanics. However, qualified undergraduate students can learn a great deal about the concepts and essential aspects of the necessary techniques for studying one of these problems. The summer project would begin with the selection by the student of a specific topic of his/her interest. During the first couple of weeks, the student will be provided background materials and will be introduced to basic computer, graphics, and mathematical techniques. The REU student will have the complete guidance from the professor and from a postdoctoral research associate, and/or advanced graduate students. As the student becomes better prepared and more familiar with the necessary background materials, he/she will be given a simple model problem to practice. After the student succeeds in reproducing the known results and has gained enough confidence, he/she will be encouraged to participate in an ongoing project in the group or even a completely new project. Previous REU students in the group have all found that the training received and the experience gained in working on a frontier and exciting chemical physics problem are very valuable to their future graduate research career.