A. Briefly describe overall research program at your laboratory.

The theme of our research is the use of computational approaches, supplemented by experimentation, to address practical yet challenging problems in the broad area of physical chemistry. Our current research focus is multifold: (1) develop new theoretical and conceptual methods and implement them in efficient computer programs, and (2) model by utilizing several analytical/spectroscopic data, and (3) apply these computational models to solve problems in chemistry. Research at our lab employs quantum mechanical (QM) modeling software, such as Spartan, Gaussian and VASP to understand/calculate molecular structure, transition state geometry and reaction coordinate, excited states of molecules, and potential energy surface. We also write computer programs to solve problems such as classical molecular dynamics, calculating reaction path, quantum dynamics of molecules. The experimental side of our research utilizes several experimental techniques such as MDSC, ITC, FTIR, UV-Vis, Raman, X-ray diffraction. Current research topics are: (a) Chemical reaction dynamics and computing reaction paths, (b) improving bioavailability of low-soluble pharmaceutical ingredients, (c) Measuring thermodynamic properties due to interactions of two chemical species by applying ITC, (d) Designing photo-chromic materials, (d) quantum dynamics of molecules interacting with laser electric field, (e) wave-packet dynamics of photo-dissociation.

B. Briefly describe specific project(s) for your teacher

Computational project: Intermolecular interaction is at the heart of all chemistry. The aim of this specific project is to identify suitable modeling scheme for quantifying intermolecular interaction between two different molecules. Calculating many-body non-bonded interaction energy is daunting task from the formulation point of view as well as computationally. The idea is to investigate the basis set superposition error (BSSE) and Counterpoise (CP) correction scheme to calculate the interaction energy. The interaction energy is related to the stability of the complex formed between any two compounds. Knowledge gained from the interaction energy and stability of the complex can then be applied to study the Polymer-drug complex, which is one of the major modes of drug delivery system currently in use in pharmaceutical industry. One of our research areas, as mentioned above, is improving bioavailability of low-soluble active pharmaceutical ingredients (API) by embedding API with a polymer; this requires detail study of the intermolecular interaction and stability of the API-polymer complex.

Despite enormous application of the QM software, accurate calculation of the interaction energy even for small molecules is a challenge. This is where this project bears importance from methodical point of view and we would, to begin with, investigate the BSSE-CP method to smaller system in order to gain understanding and applicability of the method. As we progress, the implementation will be done to API-polymer complex.
Experimental project: The experimental side of the research involves application of the isothermal titration calorimetry (ITC) and infra-red (IR) spectroscopy to determine thermodynamic properties of interaction (such as enthalpy change, entropy change, free energy change, equilibrium constant, binding constant), kinetic properties (rate constant, catalytic constant for enzyme), and spectroscopic properties (IR spectrum and frequency). The research focus in ITC is injecting one molecule into other and determine the heat of reaction due to interaction between the two molecules. The heat absorbed/released due to the interaction are then analyzed to obtain thermodynamic properties. In the spectroscopic experiment, two different chemical species are mixed and their interactions are monitored with respect to the shift in the frequency and absorbance in their IR spectra.

This will allow us to study the interaction energy (enthalpy and free energy) experimentally which can then be validated with computational modeling. At the end of this research, the candidate teacher will have enough data to publish in a Journal and present at conferences.

C. Will any other people (post docs, grad students, undergraduate students, colleagues, etc.) be involved directly with your teacher?

I will have two undergraduate students who will be working on different topics in the same lab. One chemistry professor from India will also be visiting my lab and carrying out some research during the summer. The teacher candidate will be involved in some sort of interaction with these other people, perhaps in a group discussion of individual research on a weekly basis.

D. Will you require any advanced reading/preparation for the teacher? If yes, please briefly describe.

Yes, its always helpful. I will email some relevant literatures prior to the start of the research. The research involves a good amount of mathematics (integration, differentiation, differential equation) and some physics. So it will be helpful to brush up math and physics a little bit.