Summer 2012 URP Proposal
Molecules on Graphene and Calculations of Model Nanosensors

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Graphene is a one atom thick layer of carbon in a hexagonal lattice (think nanosize chicken wire). Graphene along with diamond, graphite, carbon nanotubes, C_{60} buckyball, and other fullerenes are all forms of pure carbon. Graphite is made of a series of these graphene layers stacked atop one another. Graphene in pure form has been known only since 2004. Graphene is well known to have unique and desirable properties of electrical conductivity, thermal conductivity, transparency, high strength to density ratio, etc. Graphene also has been shown to be capable of functioning as a sensor for molecule detection. DNT (dinitrotoluene, a volatile compound present in explosives) has been detected down to a level of 28 ppb (parts per billion). Future nanosensors could operate on the change in graphene's electrical conductivity due to the adsorption of molecules on the atom thick layer of carbon atoms. An important aspect of graphene-based sensors is the ratio of gas phase composition to surface adsorption concentration. The extent of surface adsorption should be proportional to the surface binding energy. At the present time these surface binding energies are not available from experiments.

My students and I previously have used computer-based models of graphite surfaces, rough surfaces, porous surfaces, and carbon nanotubes in conjunction with molecular mechanics to calculate molecule-surface binding energies. These calculated values have been compared to experimental values obtained from gas-solid chromatography and thermal desorption. Molecule-surface binding energies for adsorption are relevant to a wide variety of practical applications including: trapping environmentally harmful molecules, recycling industrial gases, storing energy molecules, isolating chemical warfare agents, predicting molecular separations in chromatography, monitoring environmental gases, and removing objectionable odorant molecules. This summer I expect to focus on the interactions of molecules with graphene or chemically modified graphene and its role as the basis of a nanosensor device.

Our goal is to predict molecule–graphene or molecule–modified graphene surface binding energies (how strongly molecules are held on the surface) based on calculations using *Scigress*, *Gaussain*, or *Spartan* software employing molecular mechanics or quantum-approximation methods. Interesting molecules for calculations of model nanosensors could include explosive compounds, volatile explosive signature molecules, chemical warfare agents, environmental pollutants, odorants, etc. These interaction energies would be used to generate molecule-surface potential energy curves that in turn could be used to predict the extent of adsorption at low vapor concentrations. These calculations would be aimed at predicting molecule surface densities present in model nanosized sensors as a function of temperature, gas phase concentration, and molecular structure.