

Summer 2010 URP Proposal

Molecule-Carbon Surface Interactions

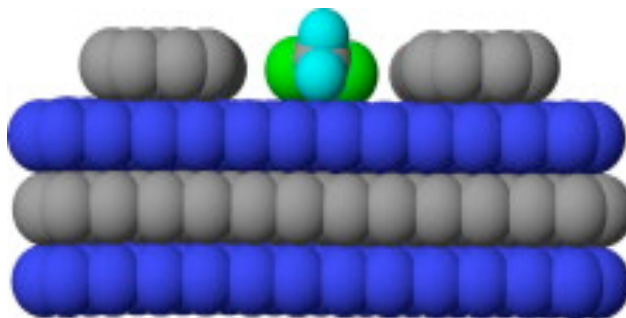
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My general area of study deals with molecule-surface interactions, and my current interests are the interactions of odorants, greenhouse gases, biological molecules, and pharmaceutical drugs with various types of porous carbon powders. Depending on student and faculty interests and the status of ongoing projects at the time this work is done, the summer research may involve laboratory work, computer-based molecular modeling, or both of these methodologies.

There are a variety of therapeutic pharmaceutical agents (drugs) that are most beneficial when released over an extended time period. There are different techniques that have been utilized to facilitate time release of medicines – encapsulation in biodegradable polymers, for example. More recently there has been an interest in mesoporous materials (usually silica based) for controlled drug release. We have begun to explore the ability of various carbon powders having macro, meso, micro, and nano porosity to hold and then gradually release retained pharmaceutical molecules. Carbon powders have good structural integrity, and span a wide range of surface area and porosity. We have studied molecule trapping and release over time ranges from hours to weeks and would like to continue this work. A simple technique such as uv/visible spectroscopy is suitable for detection and quantification. Variables of interest include temperature, pH, ionic strength, powder porosity, powder surface area, target molecule identity, loading conditions, and time.

Another area of interest is based on computer models of a variety of carbon surfaces that prior students have created using the software Scigress. We have used models of graphite surfaces, rough surfaces, porous surfaces, and carbon nanotubes in conjunction with molecular mechanics to calculate molecule-surface binding energies and compared to experimental values obtained from gas-solid chromatography and thermal desorption. These calculations are relevant to a wide variety of practical applications including: trapping environmentally harmful molecules such as super greenhouse gases, recycling industrial gases, storing energy molecules, isolating chemical warfare agents, predicting molecular separations in chromatography, monitoring environmental gases, and removing objectionable odorant molecules.

Recent students have been co-authors on articles published in the *Journal of Colloid and Interface Science*, and have presented their research at meetings of the American Chemical Society. Please see me for more information about these projects.



Side view of dichlorodifluoromethane on a rough carbon surface mode