Physical Chemistry Seminar

Tuesday, May 4, 2010 | **11:00 a.m.** | **Room 1315 Chemistry Building**

Quantum Entanglement and Born-Oppenheimer Breakdown in Chemical Reactions

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High-resolution experiments have stimulated the detailed theoretical study of elementary chemical reactions. Among the most studied are the reactions of F and Cl with molecular hydrogen. The vast majority of earlier work has assumed that reaction takes place solely on the lowest potential energy surface, as predicted by the Born-Oppenheimer approximation. In fact, low-lying electronic states will contribute to these (and many other) chemical reactions. This quantum entanglement allows the excited spin-orbit state of the halogen to react, especially at low collision energy where the reaction barrier inhibits reaction of the spin-orbit ground state.

We shall discuss how one undertakes the theoretical study of these reactions, in an attempt to elucidate the degree to which quantum mechanics plays a role in chemical reactivity. Our theoretical simulations will be compared with the results of sophisticated molecular beam experiments.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:15 p.m. in Room 8305f