Developing smaller microchips to power new electronic devices has and always will be of top priority to microchip manufacturers. The major limiting factor on the size of a microchip has been the ‘etching’ process. Etching can be thought of as carving out certain physical characteristics into the semiconductor surface which lead to the desired device physics. Before etching occurs, a ‘mask’ is developed on top of the surface in a process called lithography. The mask exposes certain regions to the etching process while protecting others. The device size is limited by the ability to transfer the mask geometry onto the semiconductor surface. Currently, etching is done by bombarding the semiconductor surface with ionized atoms. These ions remove the desired regions of the surface by momentum transfer, which physically breaks off clusters of atoms. This process leaves highly disordered layers on the semiconductor surface and results in damage to electrical and optical performance. A much better etching process would not create surface damage and could be highly selective in the regions that the developer wants removed. Such a damage free etching process has been developed by H. P. Gillis and Systine Inc was founded for further development. This much better process uses low energy electrons to etch the surface. Low energy electron enhanced etching (LE4) uses electronic excitations to remove the desired regions from the surface. The result is higher quality surfaces than can be produced by ion etching. While LE4 has become a well observed process, the mechanism that drives LE4 is not a very well understood process. The goal of this project is to use computer simulations to help develop a deeper understanding of the mechanisms behind LE4. Currently, the LE4 mechanism is hypothesized as being related to the Knotek-Feibelman mechanism (KF) for electron stimulated desorption (ESD). We have studied the initial single core hole states of this mechanism and have begun calculations on the final two hole states. Initially electrons are removed from a simple test system and Jaguar is used to calculated the forces on the atoms. The atoms are then allowed to move in response to these forces and the process is repeated. The CMDF with Open Babel interfaces has allowed these simulations to be completely Python driven.