PROJECT: Electron Transfer during Ion-Surface Collisions

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PROJECT GOAL
The goal of this research is to investigate the static charge transfer between negative hydrogen ions and silver surfaces. This includes the calculation and analysis of the projected density of states for fixed ion-surface distances, and simple elements of ion dynamics.
The projected density of states (PDOS) provides information about all the atomic and surface states involved in the interaction, including their energies and widths.

The PDOS is obtained by calculating the Fourier Transform of the Autocorrelation Function (which is the overlap between the time-propagated wave function of the electron involved in transfer, and the original ion wave function).

Electron wave functions and energies are obtained with Wave Packet Propagation methods.

The modulo squared of the Autocorrelation Function when time goes to infinity provides survival probabilities.

Calculations have been performed on UNIX workstations. All data processing and graphics was performed in Origin. The Origin software was purchased from OUR grant funds.
SUMMARY OF RESULTS:
Some of our results are summarized below:

For each ion-surface distance, the PDOS exhibits peaks associated with the energies of all states involved in the interaction (not shown). Thus, all ion, surface, and images state have been identified. Their energy variation with the ion-surface distance shows that while the image states barely change, there is an avoided crossing between the ion energy (in black) and the silver surface state energy (in blue). This avoided crossing will affect the ion survival. It will help explain the experimental ion fractions. This will be the next step of this research.