

My Long Personal and Scientific Association with Frank Harris

I believe that it was in 1960 or 1961 that I attended a conference that had a collection of papers from Roothaan's group at Chicago on small diatomic molecules. At that conference, Frank gave a talk on some calculations on LiH. He showed that the approach that he was taking permitted proper dissociation and useful thermochemistry, unlike that available from current SCF studies.

Obviously, I was impressed and asked Frank if he would like to visit our laboratories at UTRC. I have forgotten when we first got together in East Hartford, probably in 1961/1962. Frank was deeply impressed with UTC computational facilities, which at the time were the largest industrial installation in the U.S. Boeing soon after moved to first place. This was the beginning of my long association with Frank Harris. We began by improving on the codes that Frank had developed with Howard Taylor for diatomic molecules. Our first paper together on MO Studies of Excited States of Helium was published in 1963.

In 1965, Frank and I published our first paper on using STO's in multicenter polyatomic studies. Frank's life became complicated for a few years and I invited him to take a sabbatical at UTRC for 6 months or so, I believe in 1966. He quickly moved into a new area, electron scattering, after discussions with a resident scientist, Hugh Williamson, who had been a student of Al Matsen. Frank soon developed an expansive approach to electron-atom scattering that is computationally simple and efficient.

After his sabbatical at UTRC, Frank attracted probably his most productive and brilliant student, Fritz Schaefer. In 1968, they wrote their first paper on the stability of the nitrogen negative ion. Fritz worked with Frank and I on improvements to the DIATOM code, generalizing it to handle complex spin and symmetry restrictions. Shortly after this, Frank began working with Hank Monkhorst, mainly on solid state problems. This collaboration continues today and may be the longest in Frank's history.

Frank and I have been close friends for over 50 years. We have published many papers together, traveled together in the U.S. and Europe, and offered helping hands in difficult personal times. Frank is clearly one of my best friends and I hope that we continue to see his imaginative and productive activities for many years to come.

Harvey Michels