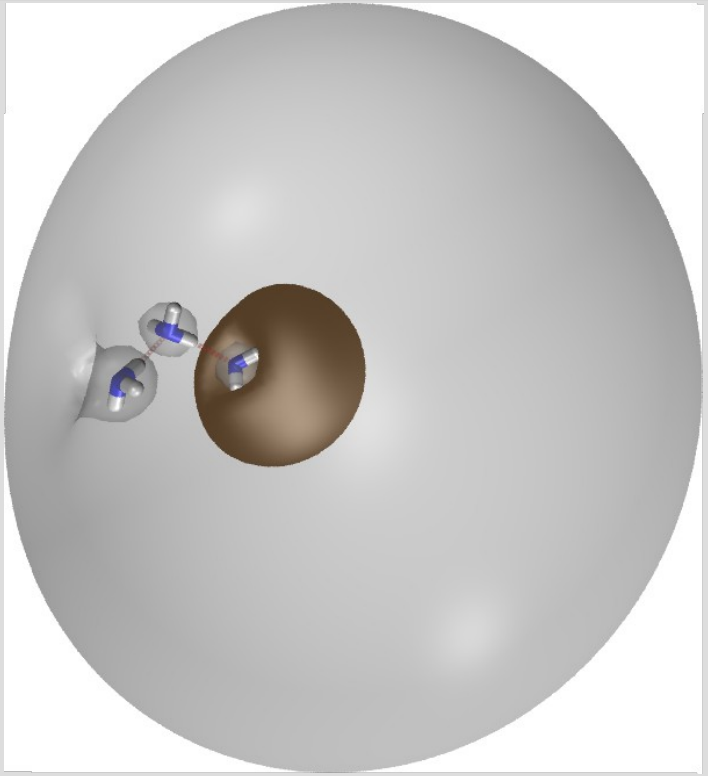
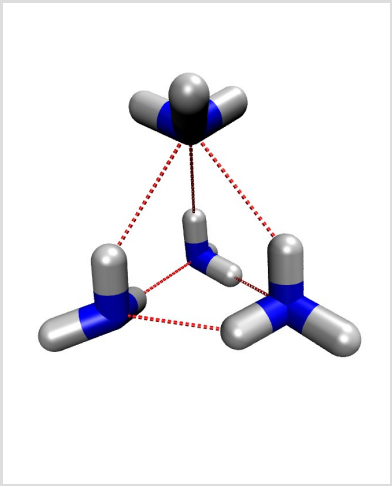
Excess electrons bound to ammonia clusters and nano droplets: Ab initio calculations, model development, and simulation.

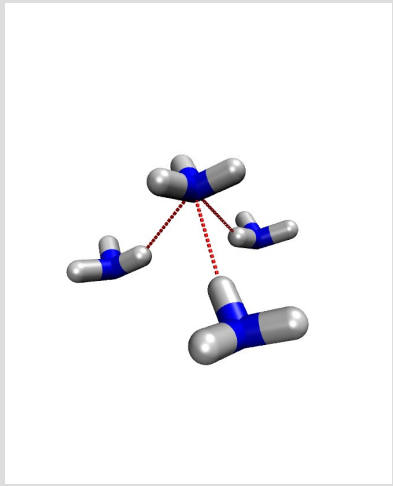
Thomas Sommerfeld, Southeastern Louisiana University

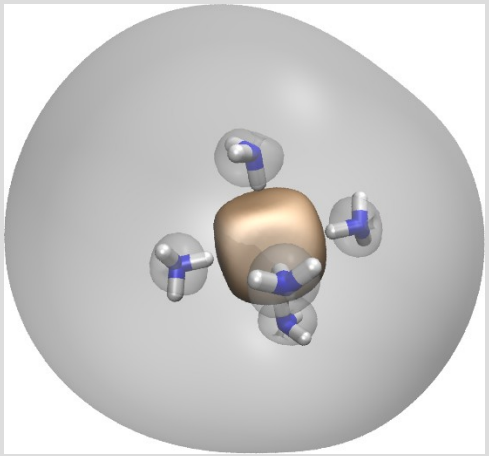


The smallest ammonia cluster able to bind an excess electron is the trimer. The binding energy is small (25 meV) and the distribution of the excess electron dwarfs the molecular framework. Iso-surfaces enclosing 10% (orange) and 80% (gray) are shown.

Small ammonia clusters need to arrange so as to form structures with large dipoles to bind excess electrons:







Small clusters do not provide good models for the ammoniated electron: This is a proposed cavity model made from six ammonia molecules. Only 20% of the excess electron's density (orange iso-surface) are inside the cavity. The 80% iso-surface (gray) is much larger than the model structure itself.