STABILITY AND DECAY OF MULTIPLY ANIONIC METAL CLUSTERS

Constantine Yannouleas and Uzi Landman
School of Physics
Georgia Institute of Technology, Atlanta, Georgia 30332-0430

The second electron affinities ($A_2$) allow for the determination of the appearance sizes of dianionic metal clusters, since electron autodetachment (which occurs for clusters with $A_2 < 0$) is the dominant decay channel over fission in the case of doubly anionic metal clusters [1,2,3].

Second electron affinities of Au$_N$ and Ag$_N$ clusters were calculated [3] using the shell-correction method and allowing for triaxial deformations. They exhibit pronounced shell effects in agreement with measured abundance spectra [4] for Au$_N^{2-}$ ($N < 30$), with appearance sizes 12 and 24 for the gold and silver dianions, respectively.

Here, we calculate the third electron affinities ($A_3$) allowing for triaxial shapes and using the shell-correction method [1,2,5]. Triply anionic clusters with $A_3 < 0$ are again unstable against electron emission. In the case of gold clusters, the third electron affinities are plotted below. In this case, the appearance size for Au$_N^{3-}$ occurs at $N \approx 60$. Notice that the major shell closure at 58 electrons creates an island of stability (the clusters with $N = 54, 55$ have $A_3 > 0$) in front of the main stability branch (with $N \geq 63$).

![Graph showing $A_3$ vs. $N$ for Au clusters with $T = 300$ K.](image)