Gas phase clusters


Seeded supersonic nozzle for the production of alkali metal clusters.

Also gas aggregation, laser vaporization, pulsed arc ...
Gas phase clusters


Size selection of the clusters can be performed by adding charge to the clusters (ionization, electron addition) followed by passing through a quadrupole, or through a B-E sector ...

![Quadrupole Mass Filter](image)

**FIG. 13.** Quadrupole mass filter. Only cluster ions with a charge-to-mass ratio corresponding to the applied ac and dc voltages will pass through the filter, as shown schematically.
Gas phase clusters


Na cluster abundance, and modeling thereof using an jellium and ellipsoidal shell models
Gas phase clusters


Abundance spectroscopy of Na and K. Because Na and K are both monovalent, their cluster stabilities are similar.
Gas phase clusters


Cu and Ag show a different set of abundances from Na and K, but maxima occur at the same positions.

For much larger clusters, supershells of stability are observed.
Gas phase clusters


Photoelectron spectroscopy allows the binding energies of electrons in clusters to be monitored: A direct measure of the electronic energy levels.

\[ h\nu = \phi + \frac{1}{2}mv^2 \]
Gas phase clusters


The energy needed to transfer an electron from one atom to another in a condensed aggregate amounts to $IP - EA$; $IP$ is the ionization energy, $EA$ is the electron affinity. The difference is the Hubbard gap, $U > 0$.

Increasing density increases wavefunction overlap as well as polarizability and therefore the screening.

Goldhammer (1913) and Herzfeld (1927) the “polarization catastrophe” occurs if the volume per atom in the material becomes smaller than the atomic

Polarizability:

$$n_C^{1/3} a_H \approx 0.38$$

Mott (1961) from Thomas-Fermi screening:

$$n_C^{1/3} a_H \approx 0.25$$
Gas phase clusters


Nano

The Kubo gap is the energy gap between (nearly) discrete energy levels in a small particle. For electrical conduction, this gap should be of the order of the thermal energy:

\[ k_B T \approx \pm \approx \frac{4E_F}{3N} \]

For a 2.4 nm Na cluster with about 170 atoms, the gap is near 300 K.

Whether a nanoparticle (or cluster) is a metal or not depends on the temperature!
Gas phase clusters


The transition from atoms to clusters to bulk phases.
Gas phase clusters


Photoelectron spectra of Na$_N^-$ clusters in the gas phase. The shell structure is visible in the larger clusters.
Gas phase clusters


Photoelectron spectra of Hg$_n^-$ clusters in the gas phase.
Gas phase clusters


The Dzugutov pair potential:

\[ V(r) = A(r^{-m} - B) \exp\left(\frac{c}{r-a}\right) \Theta(a - r) \]
\[ + B \exp\left(\frac{d}{r-b}\right) \Theta(b - r) \]

Alows polyterahedral (topologically close-packed) structures to form.
Gas phase clusters


The relaxed structures for different numbers of atoms.

The disclination networks look like stable hydrocarbons: