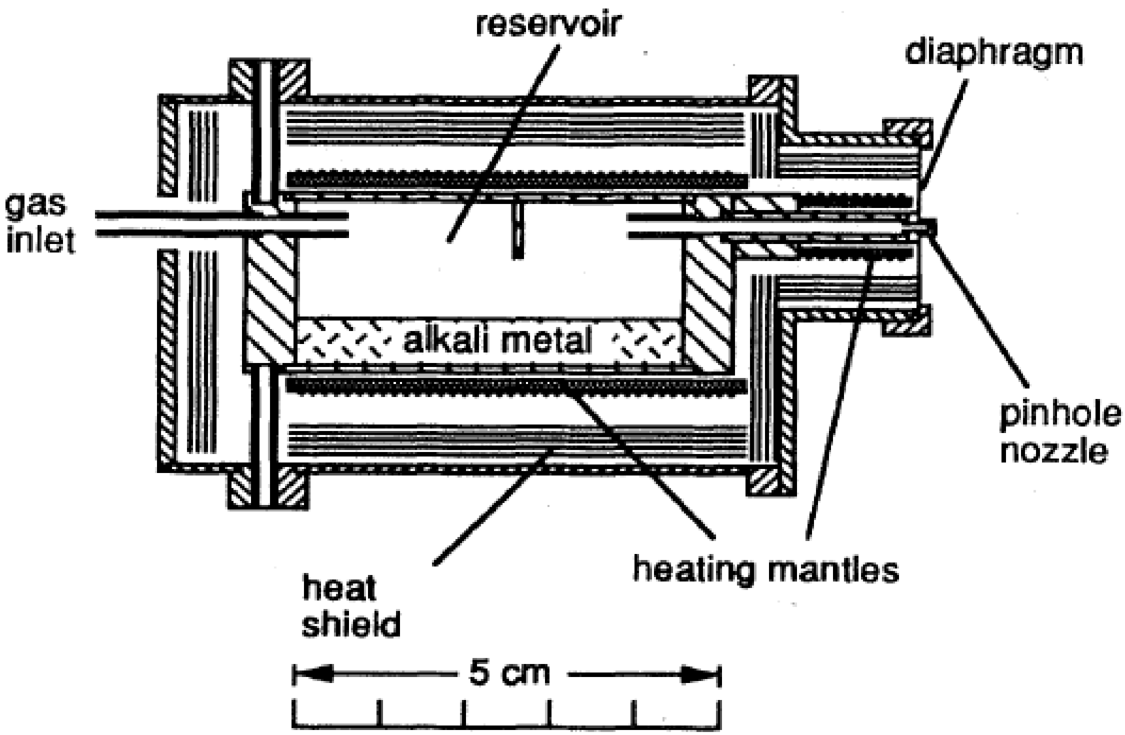
The physics of simple metal clusters: Experimental aspects and simple models, W. A. deHeer, *Rev. Mod. Phys.* **65** (1993) 611.



Seeded supersonic nozzle for the production of alkali metal clusters.

Also gas aggregation, laser vaporization, pulsed arc …

The physics of simple metal clusters: Experimental aspects and simple models, W. A. deHeer, *Rev. Mod. Phys.* **65** (1993) 611.

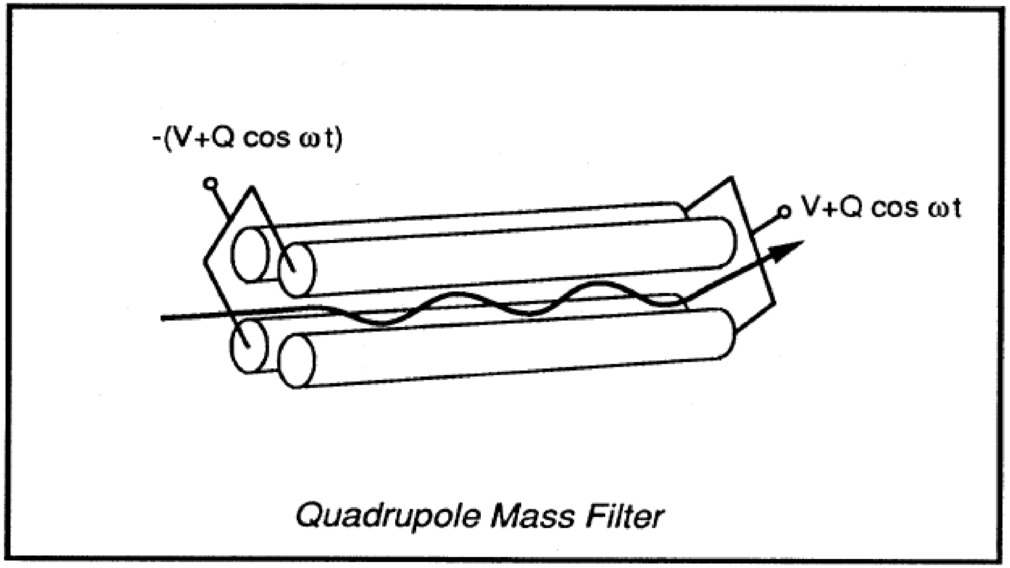
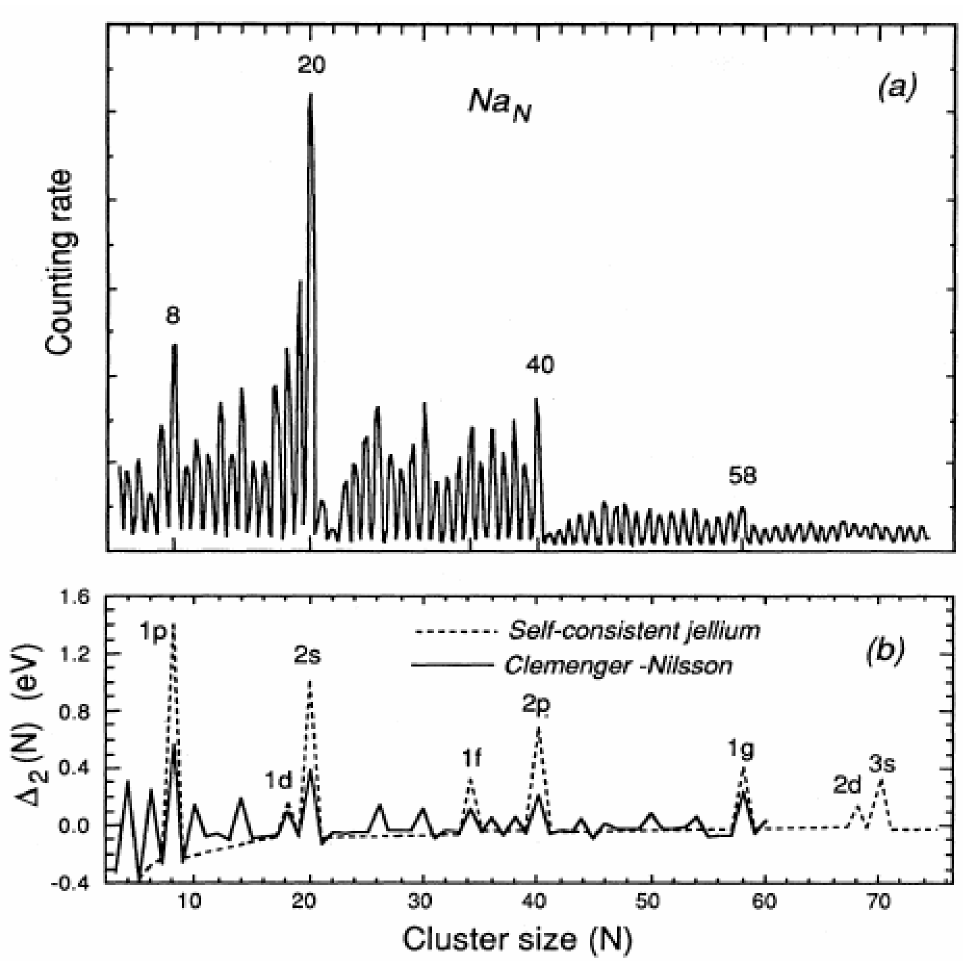


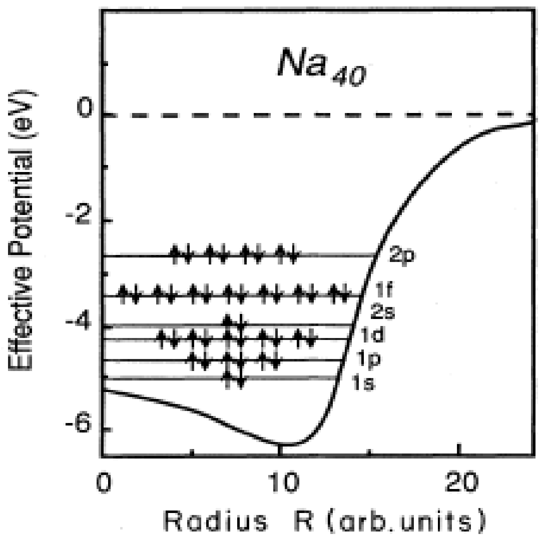
FIG. 13. Quadrupole mass filter. Only cluster ions with a charge-to-mass ratio corresponding to the applied ac and dc voltages will pass through the filter, as shown schematically.

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

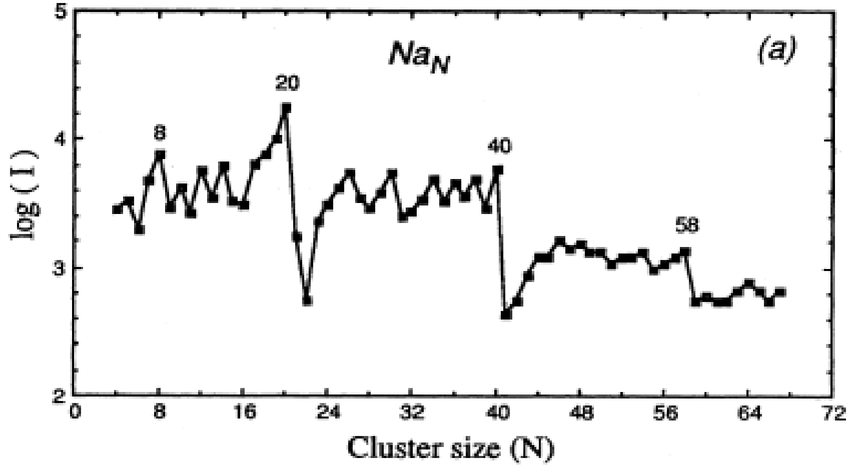
The physics of simple metal clusters: Experimental aspects and simple models, W. A. deHeer, *Rev. Mod. Phys.* **65** (1993) 611.

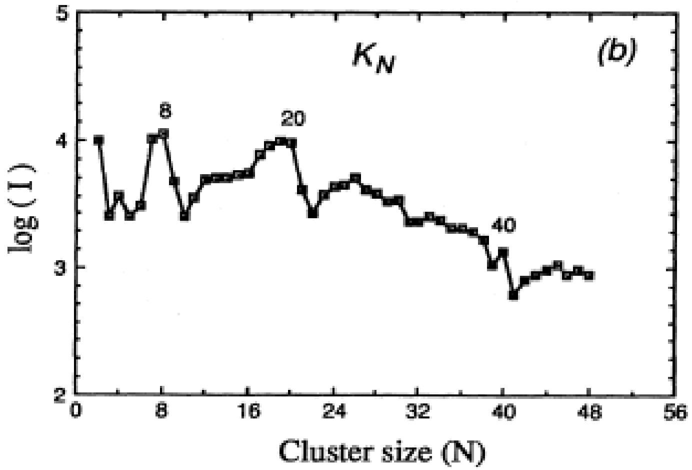


Na cluster abundane, and modeling thereof using an jellium and ellipsoidal shell models



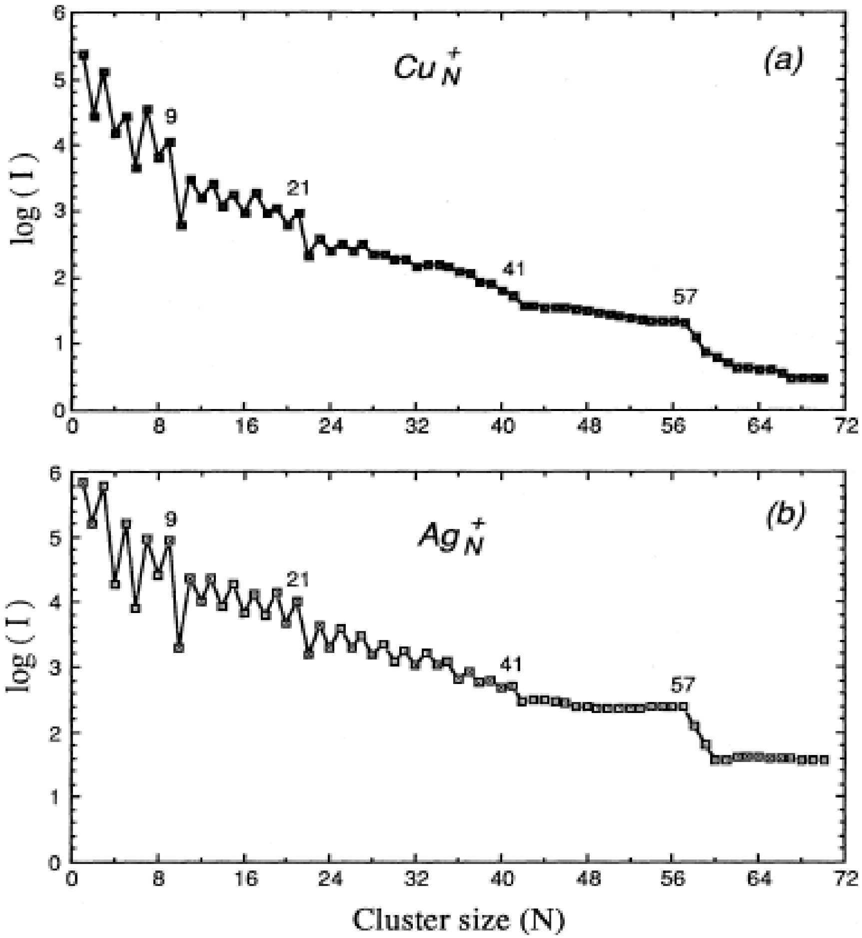
The physics of simple metal clusters: Experimental aspects and simple models, W. A. deHeer, *Rev. Mod. Phys.* **65** (1993) 611.





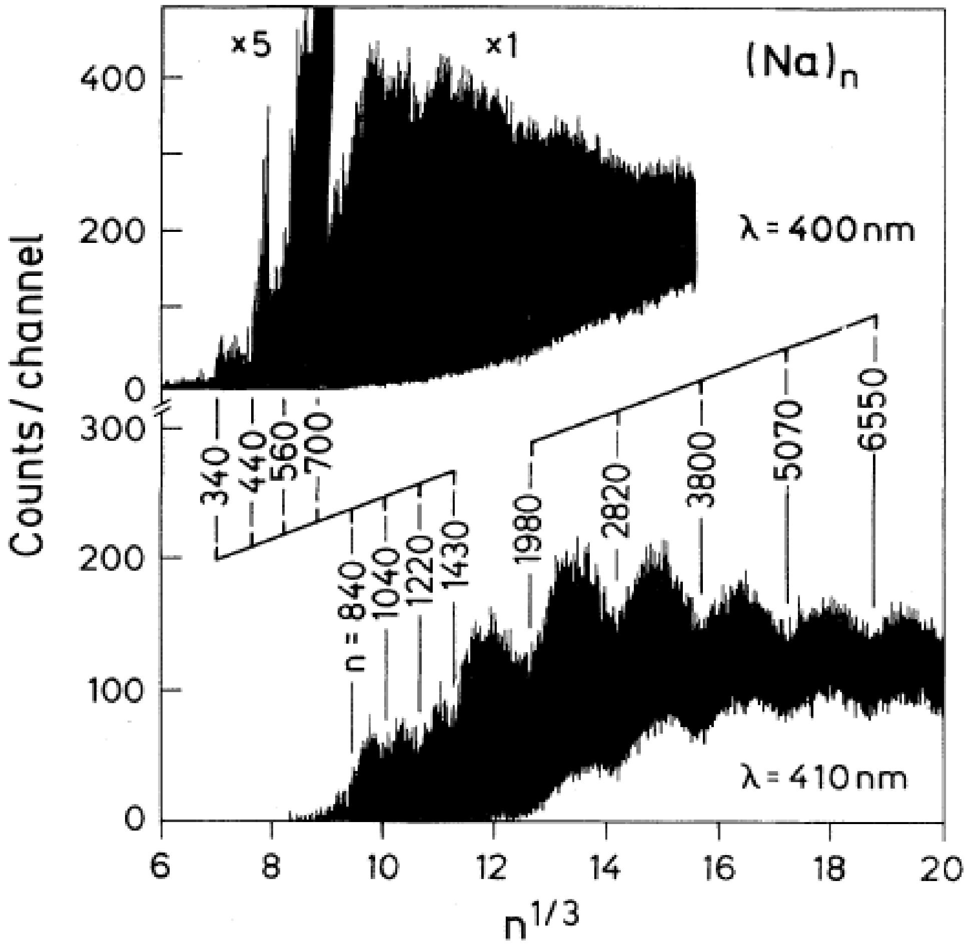
Abundance spectroscopy of Na and K. Because Na and K are both monovalent, their cluster stabilities are similar.

The physics of simple metal clusters: Experimental aspects and simple models, W. A. deHeer, *Rev. Mod. Phys.* **65** (1993) 611.



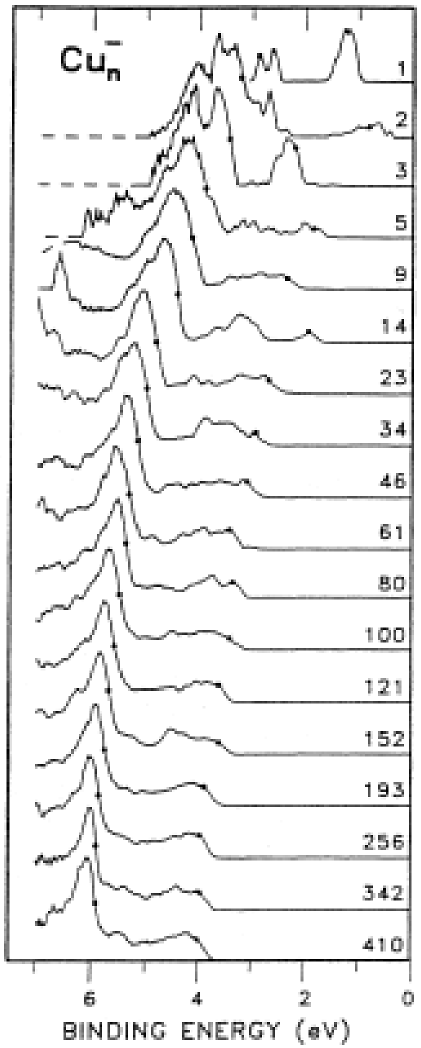
Cu and Ag show a different set of abundances from Na and K, but maxima occur at the same positions.

The physics of simple metal clusters: Experimental aspects and simple models,
W. A. deHeer, *Rev. Mod. Phys.* **65** (1993) 611.



For much larger clusters, supershells of stability are observed

The physics of simple metal clusters: Experimental aspects and simple models, W. A. deHeer, *Rev. Mod. Phys.* **65** (1993) 611.



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

$$h\nu = \phi + \frac{1}{2}mv^2$$

Metal to insulator transitions in clusters, Issendorff and Cheshnovsky, *Annu. Rev. Phys. Chem.* **56** (2005) 549.

BULK

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 therefire 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:

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

Metal to insulator transitions in clusters, Issendorff and Cheshnovsky, *Annu. Rev. Phys. Chem.* **56** (2005) 549.

Nano

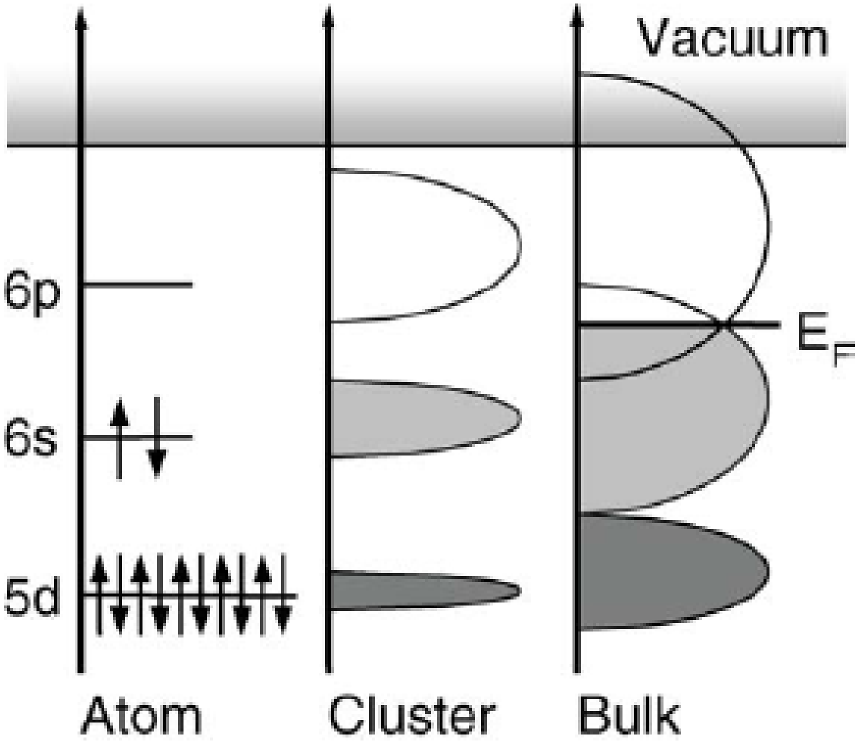
The Kubo gap is the energy gap between (nearly) discrete energy levels in a small particle. For electrical conduction, this gap should be of the order of the thermal energy:

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

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 !

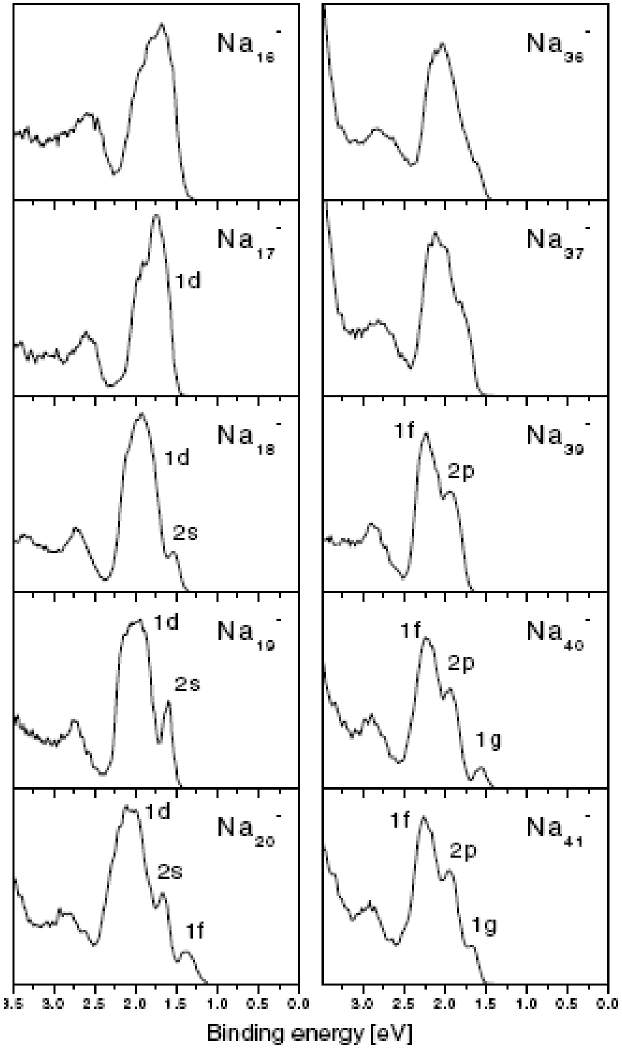
Metal to insulator transitions in clusters, Issendorff and Cheshnovsky, *Annu. Rev. Phys. Chem.* **56** (2005) 549.



The transition from atoms to clusters to bulk phases.

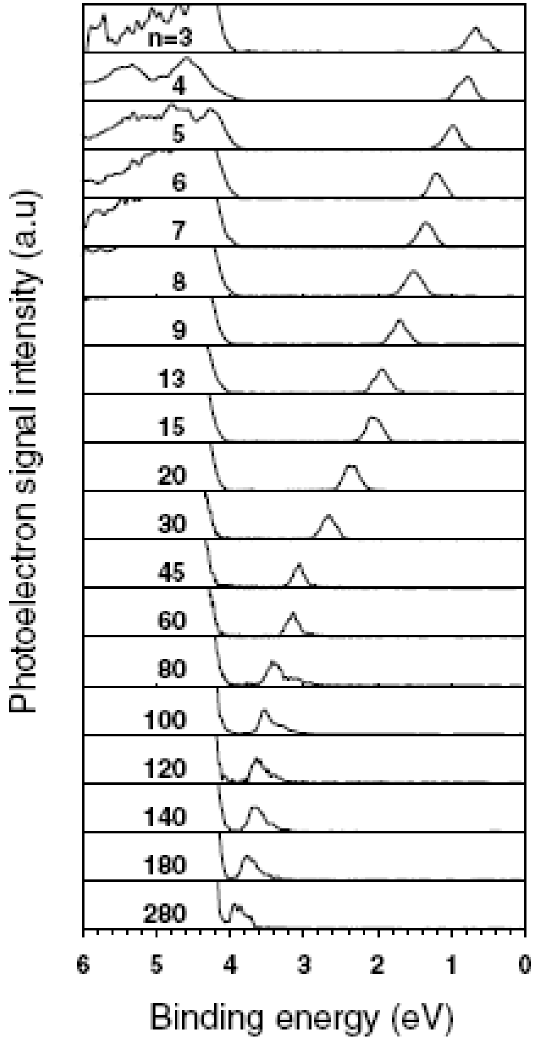
Gas phase clusters

Metal to insulator transitions in clusters, Issendorff and Cheshnovsky, *Annu. Rev. Phys. Chem.* **56** (2005) 549.

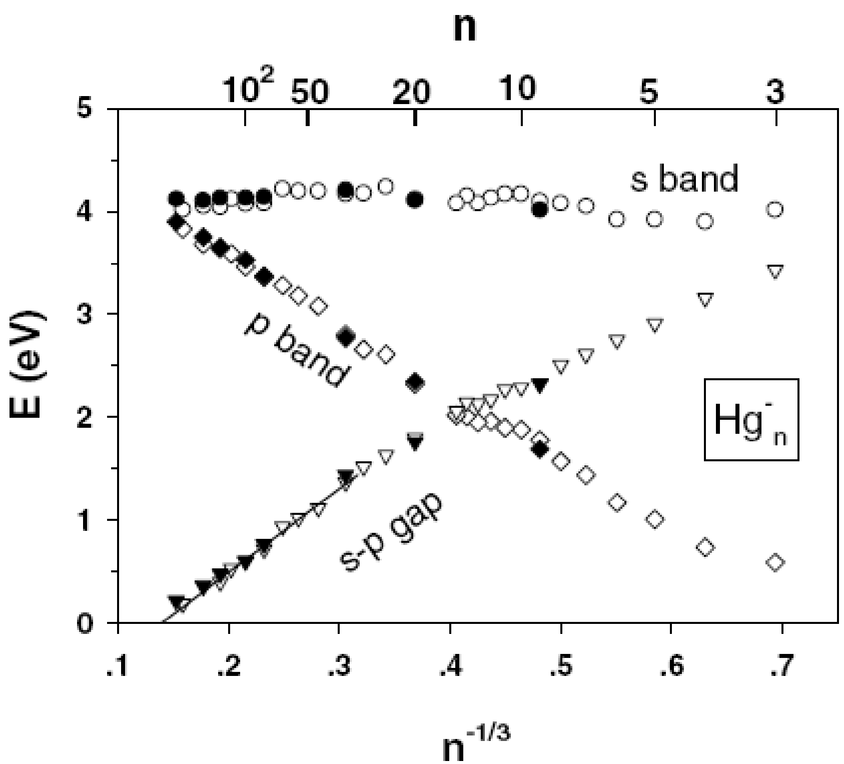


Photoelectron spectra of Na_N^- clusters in the gas phase. The shell structure is visible in the larger clusters.

Metal to insulator transitions in clusters, Issendorff and Cheshnovsky, *Annu. Rev. Phys. Chem.* **56** (2005) 549.



Photoelectron spectra of Hg_N^- clusters in the gas phase.



Polyterahedral clusters, Doyle and Wales, *Phys. Rev. Lett.* **86** (2001) 5719.

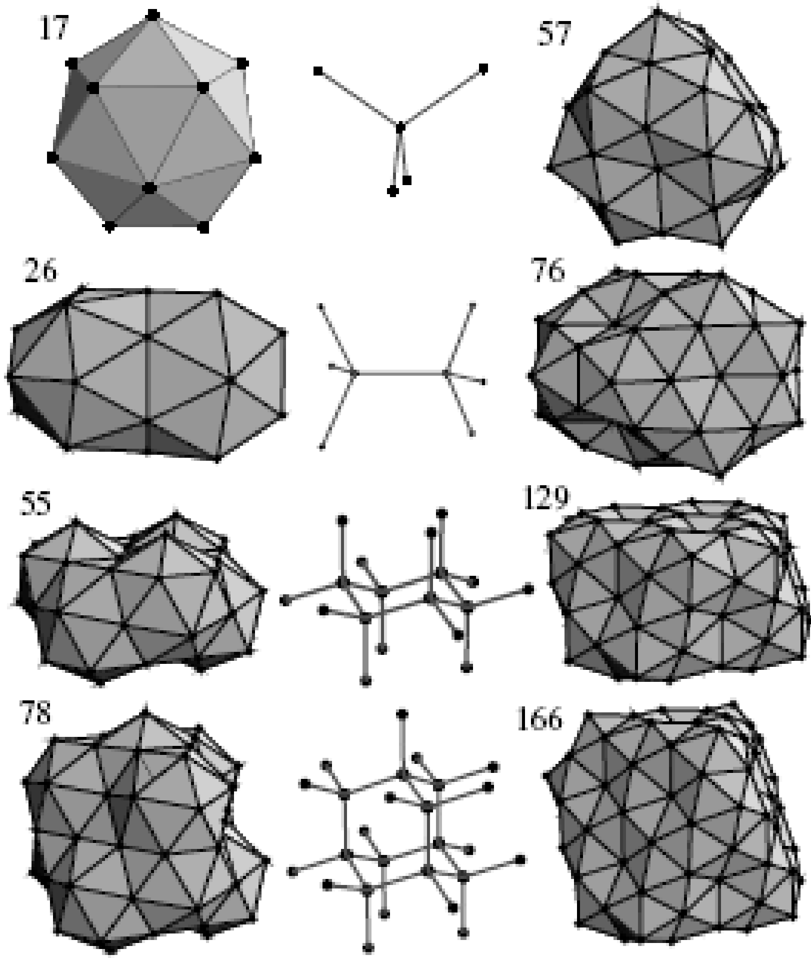
The Dzugutov pair potential:

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

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

Gas phase clusters

Polyterahedral clusters, Doyle and Wales, *Phys. Rev. Lett.* **86** (2001) 5719.



The relaxed structures for different numbers of atoms.

The disclination networks look like stable hydrocarbons: