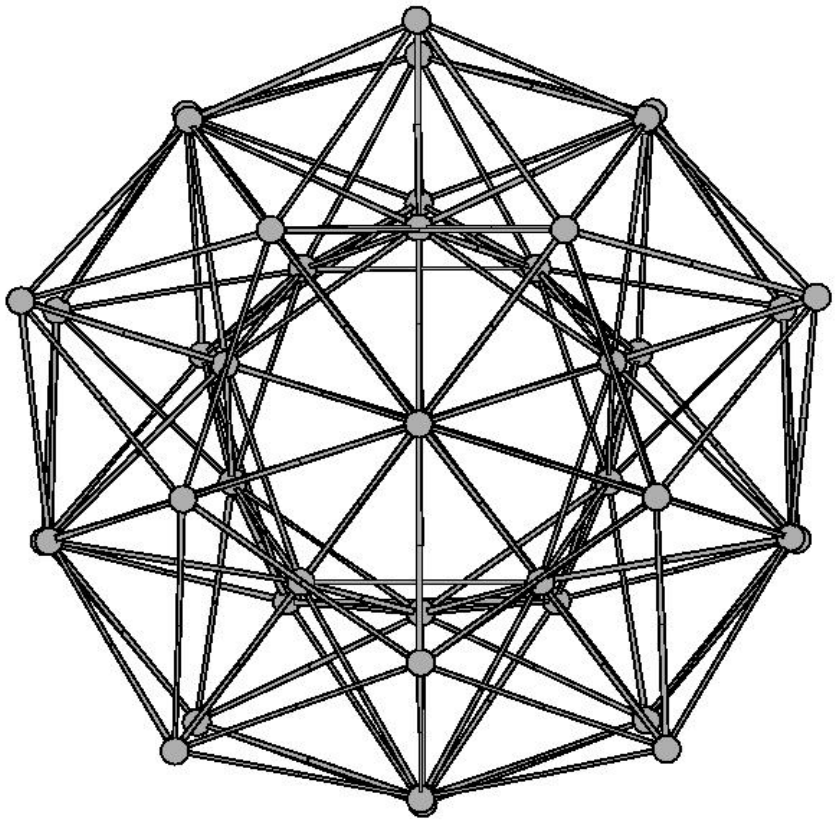
# METALLIC CLUSTERS DEPOSITED ON SURFACES



## Metallic Clusters Deposited on Surfaces

Ions, electrons, effective charges $z_i^*$

Spherical symmetry, $s$-orbitals; $d, f$-orbs, approximately

Metallic ions, point-like ($z_{Fe}^* = 0.57$,$z_{Na}^* = 0.44$)

Self-consistent potential

$$\varphi = \sum_{i=1}^{N} \frac{z_i^*}{|\mathbf{r} - \mathbf{R}_i|} e^{-q|\mathbf{r}-\mathbf{R}_i|}$$

Electron density $n = q^2\varphi/4\pi$

Potential energy, minimizataion

$$E_{pot} = -\frac{3}{4}q\sum_{i=1}^{N} z_i^{*2} + \frac{1}{2}\sum_{i\neq j=1}^{N} \Phi(R_{ij})$$

Effective inter-ionic potentials

$$\Phi(R_{ij}) = -\frac{1}{2}qz_i^* z_j^*(1 - \frac{2}{qR_{ij}})e^{-qR_{ij}}$$

Quasi-classical energy $E_q = E_{kin} + E_{pot}$,

minimization$\rightarrow q$

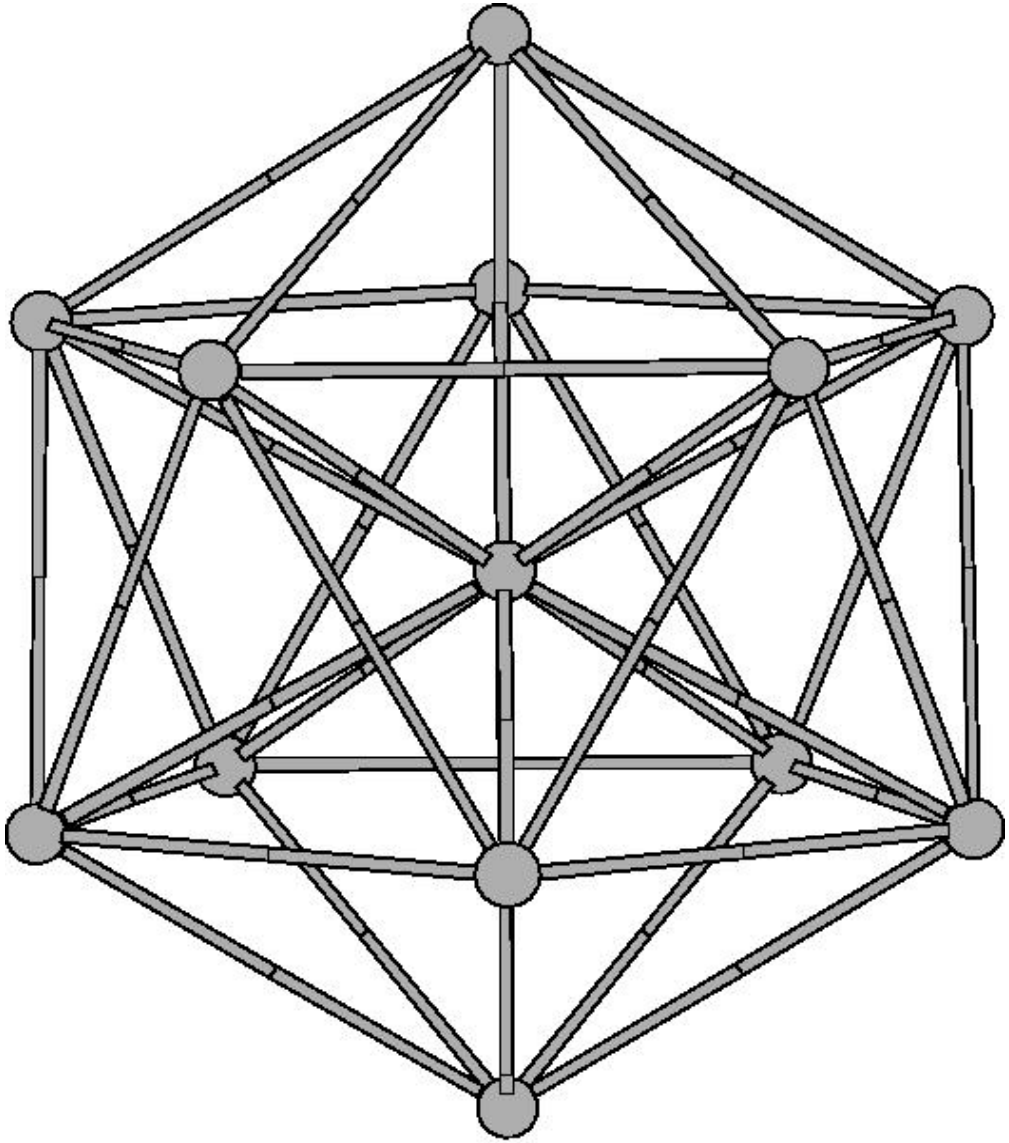
$E_{kin} = (27\pi^2/640)q^4 \sum_i z_i^*$

Screening wavevector $q = 0.77 z^{*1/3}$

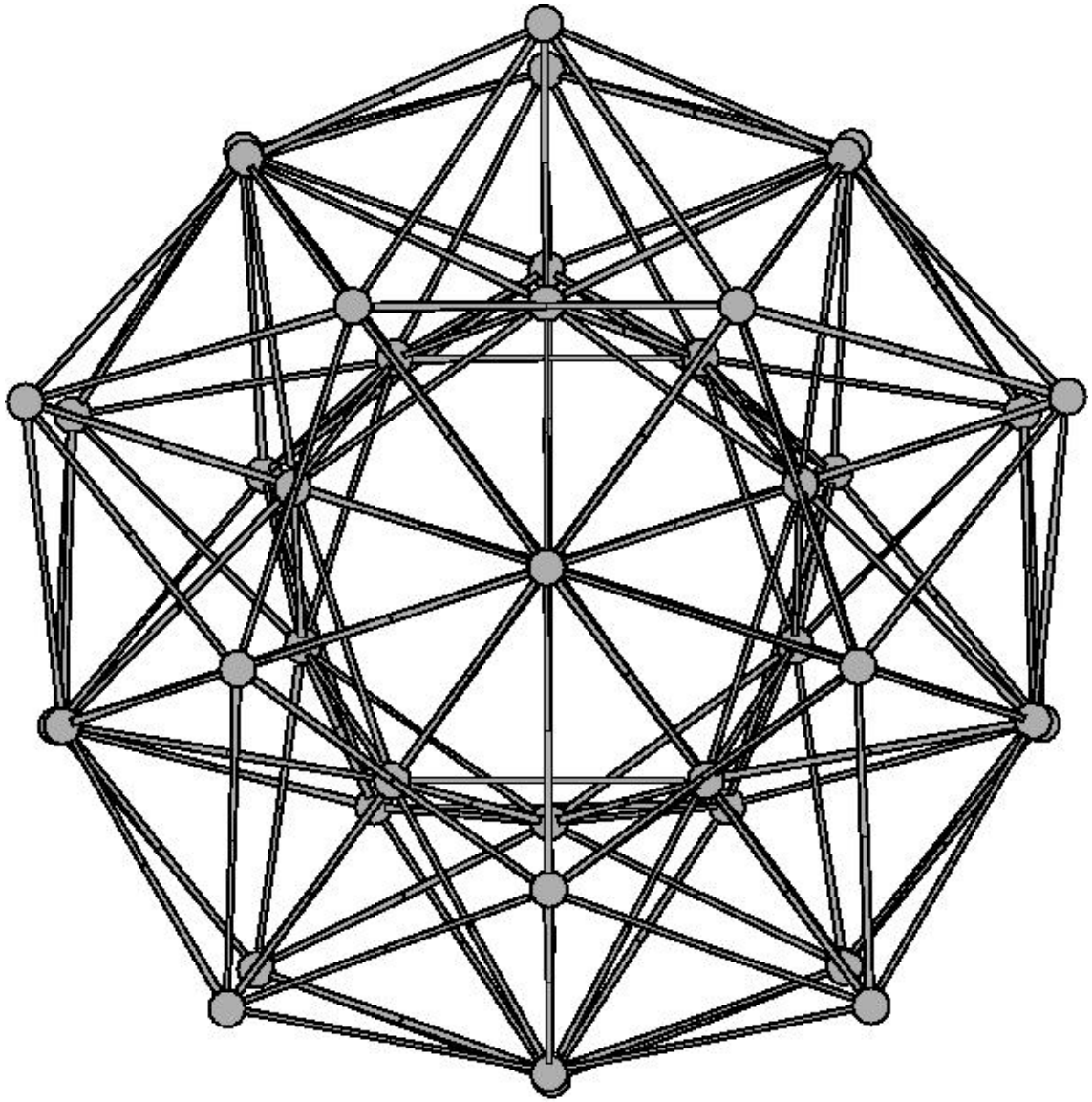
Average inter-ionic distances $a = \overline{R}_{ij} \sim 2.73/q$

Binding energy $E = E_q + E_{ex}$,

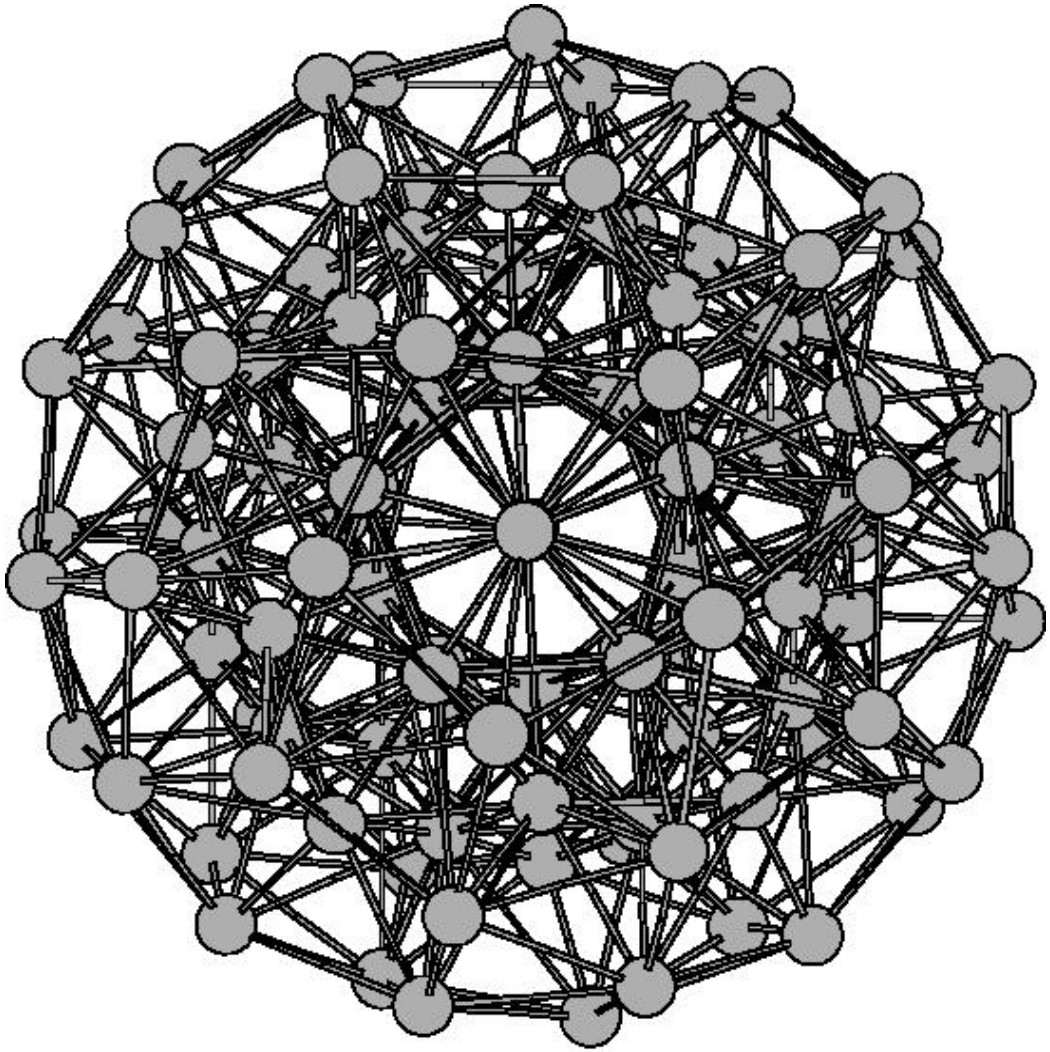
$E_{ex} = -(9/32)q^2 \sum_i z_i^*$



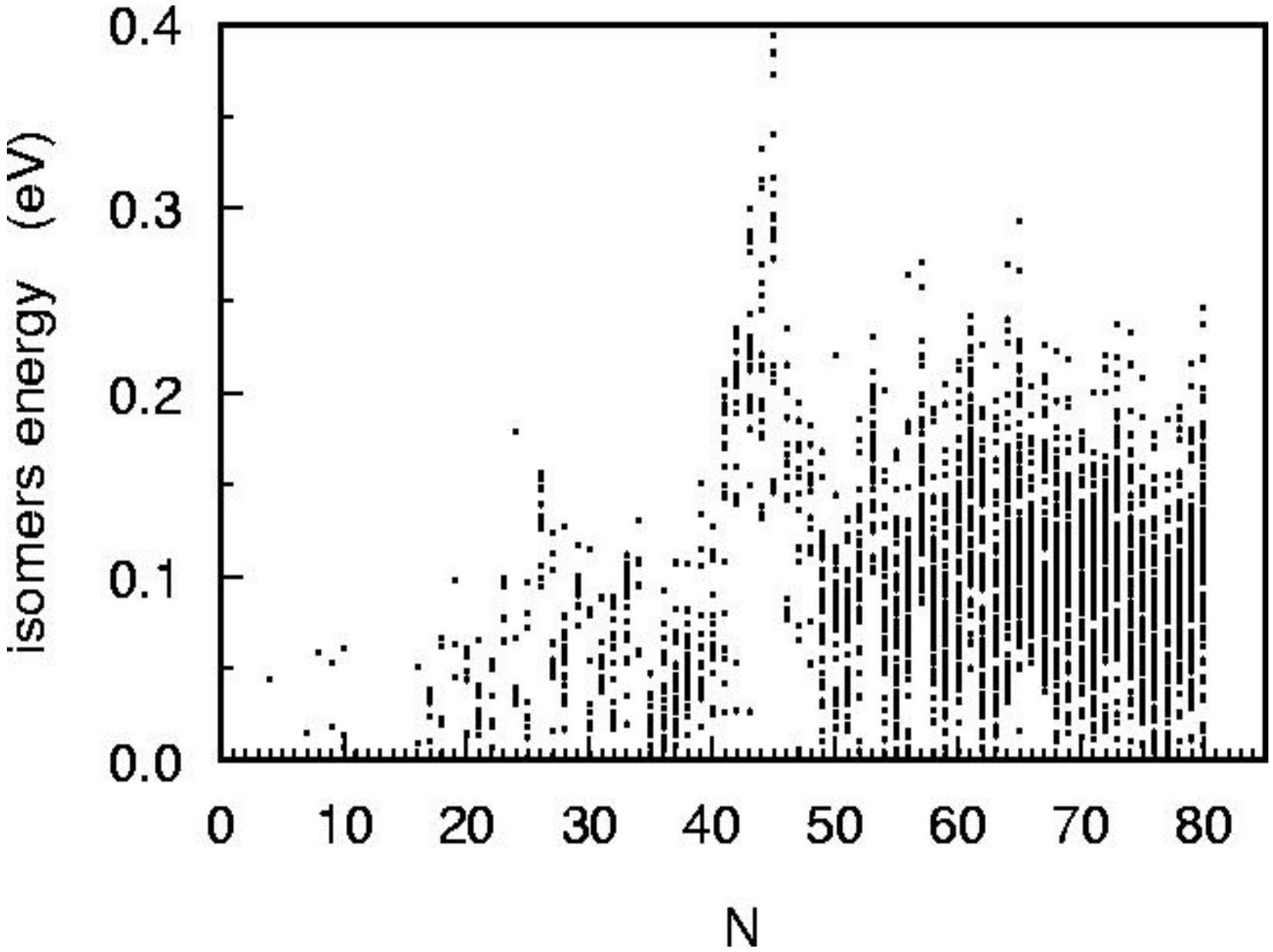
N=13

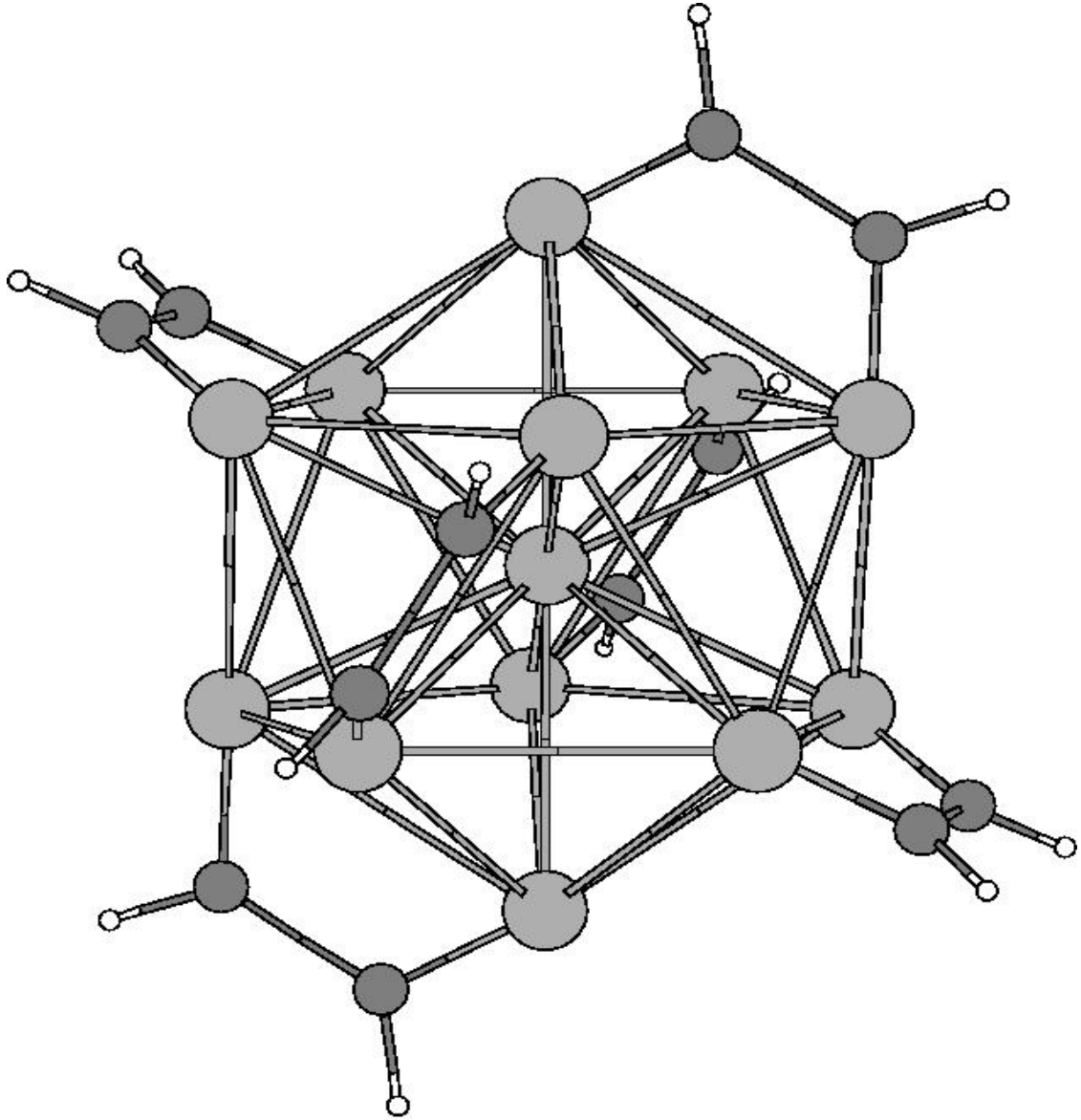


N=45

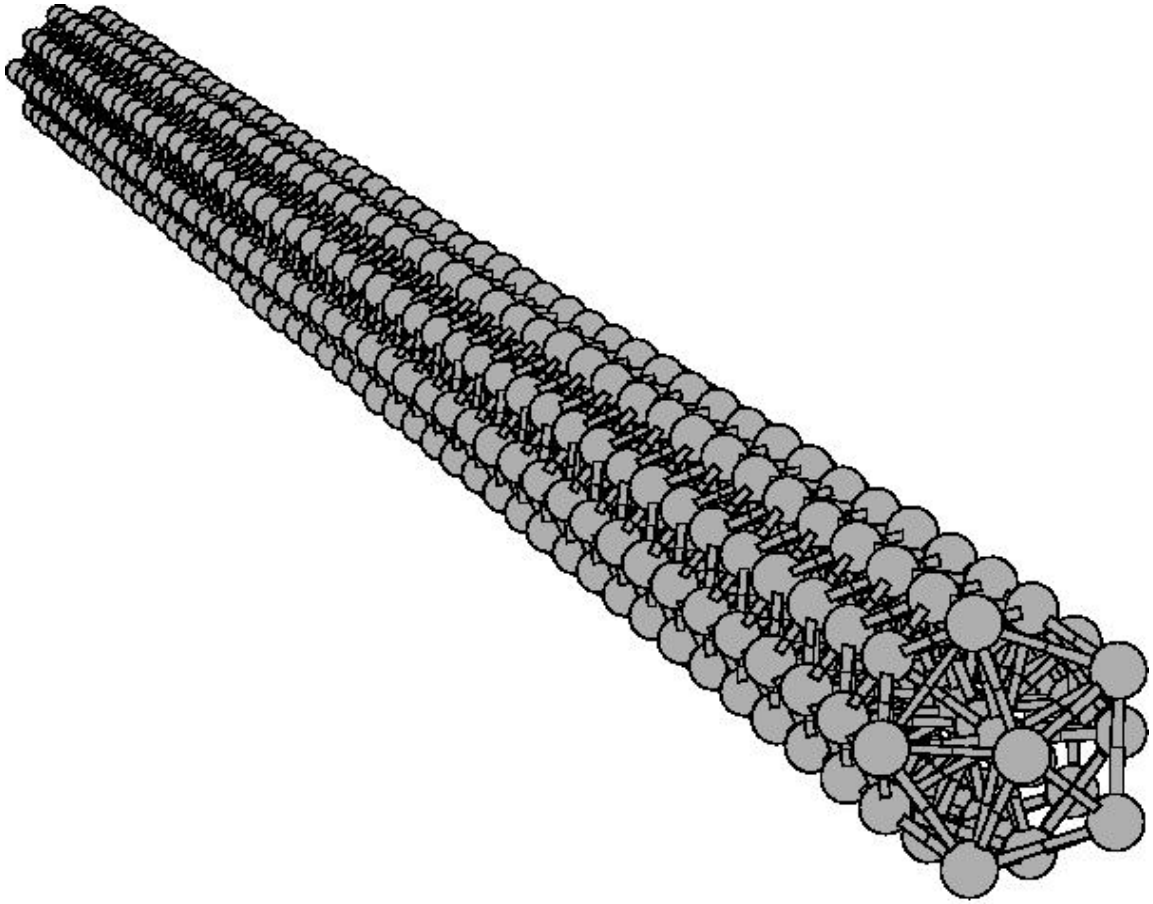


N=115

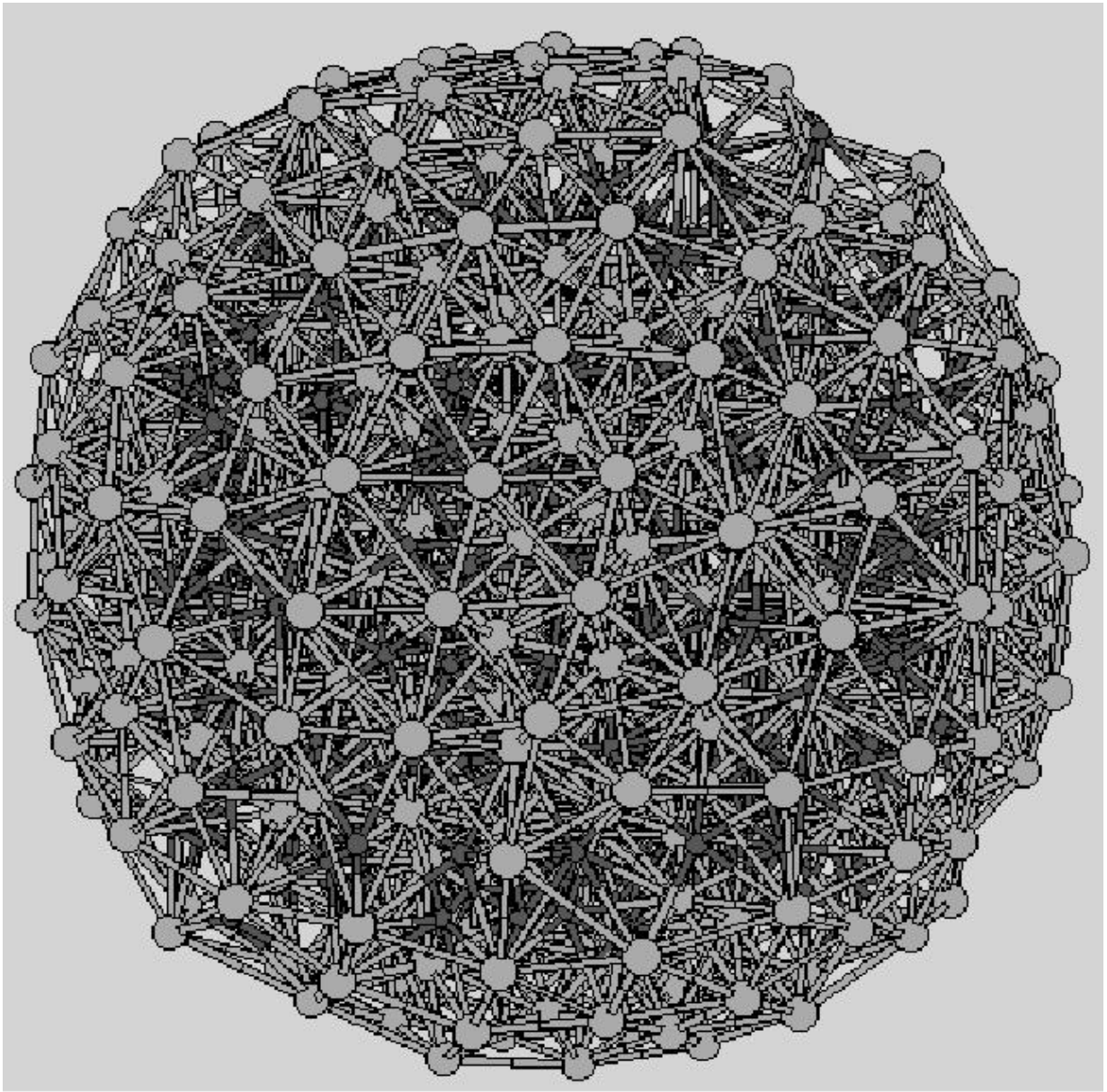

0.4
0.3
0.2
0.1
0.0
isomers energy (eV)
0
10
20
30
40
50
60
70
80
N



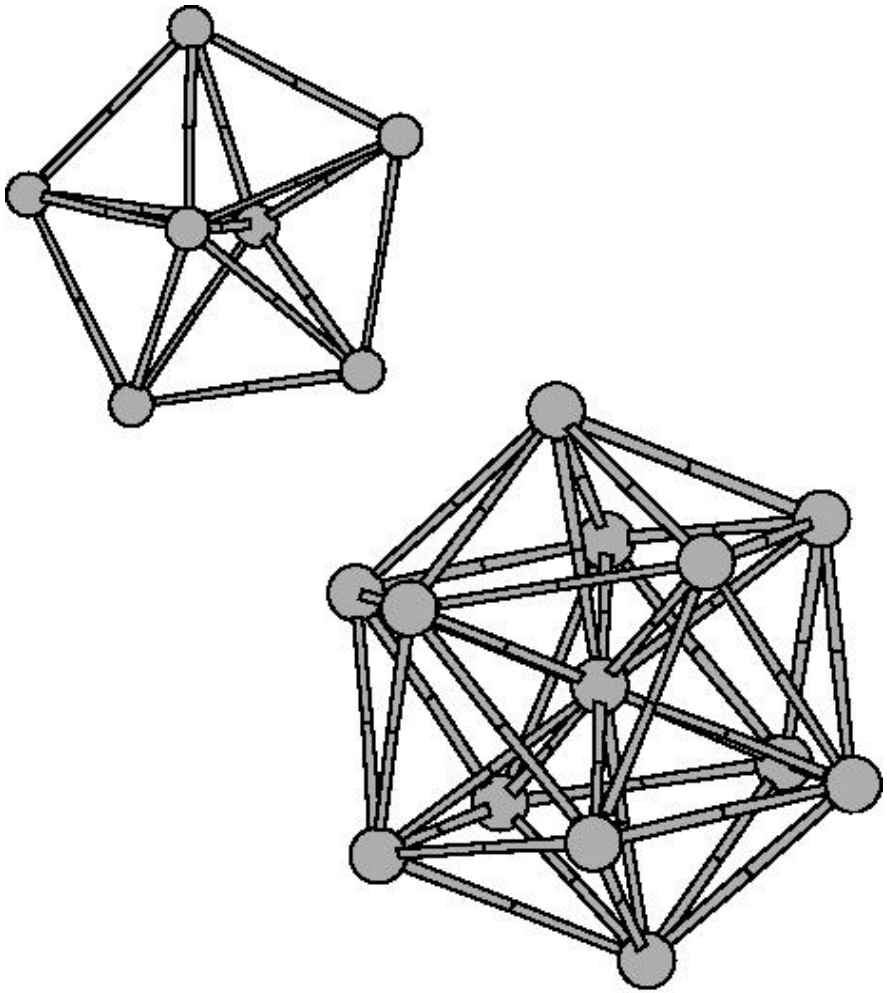
$Fe_{13}(C_2H_2)_6$



Metallic Nanowire



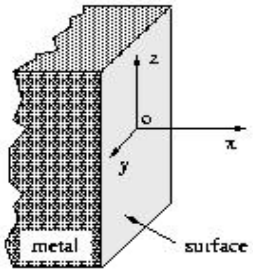
N=855

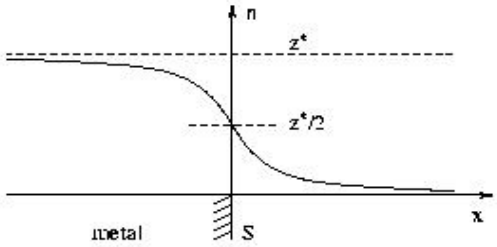


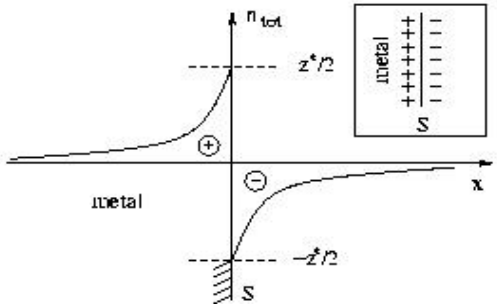
Two Interacting Clusters

Separability, Solid + ad-Atoms, their interaction

Surface potential (continuum solid)

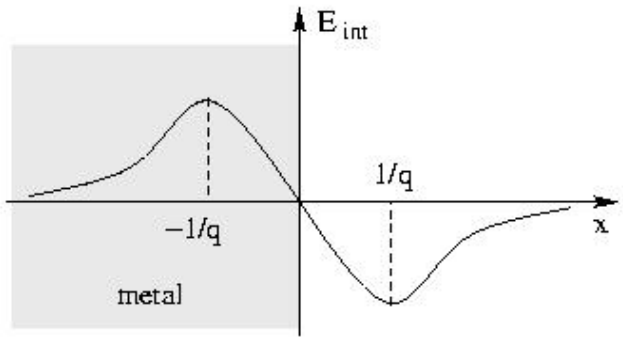


Solid-Ion interaction potential

$$E_{int} = -\frac{\pi z^* z_0^*}{q a^3} x e^{-q|x|}$$




Potential energy

$$E_{pot} = -\frac{3}{4} q z^{*2} N + \frac{\pi z^{*2}}{2 q^3 a^6} A$$

Surface tension

Semi-infinite solid + Atoms

$$E_{pot} = E_{sol} - \frac{3}{4} q \sum_i z_i^{*2} + \frac{1}{2} \sum_{i \neq j} \Phi(R_{ij}) -$$

$$- \frac{\pi z^*}{q a^3} \sum_i z_i^* X_i e^{-q|X_i|}$$

Screening wavevector of the solid

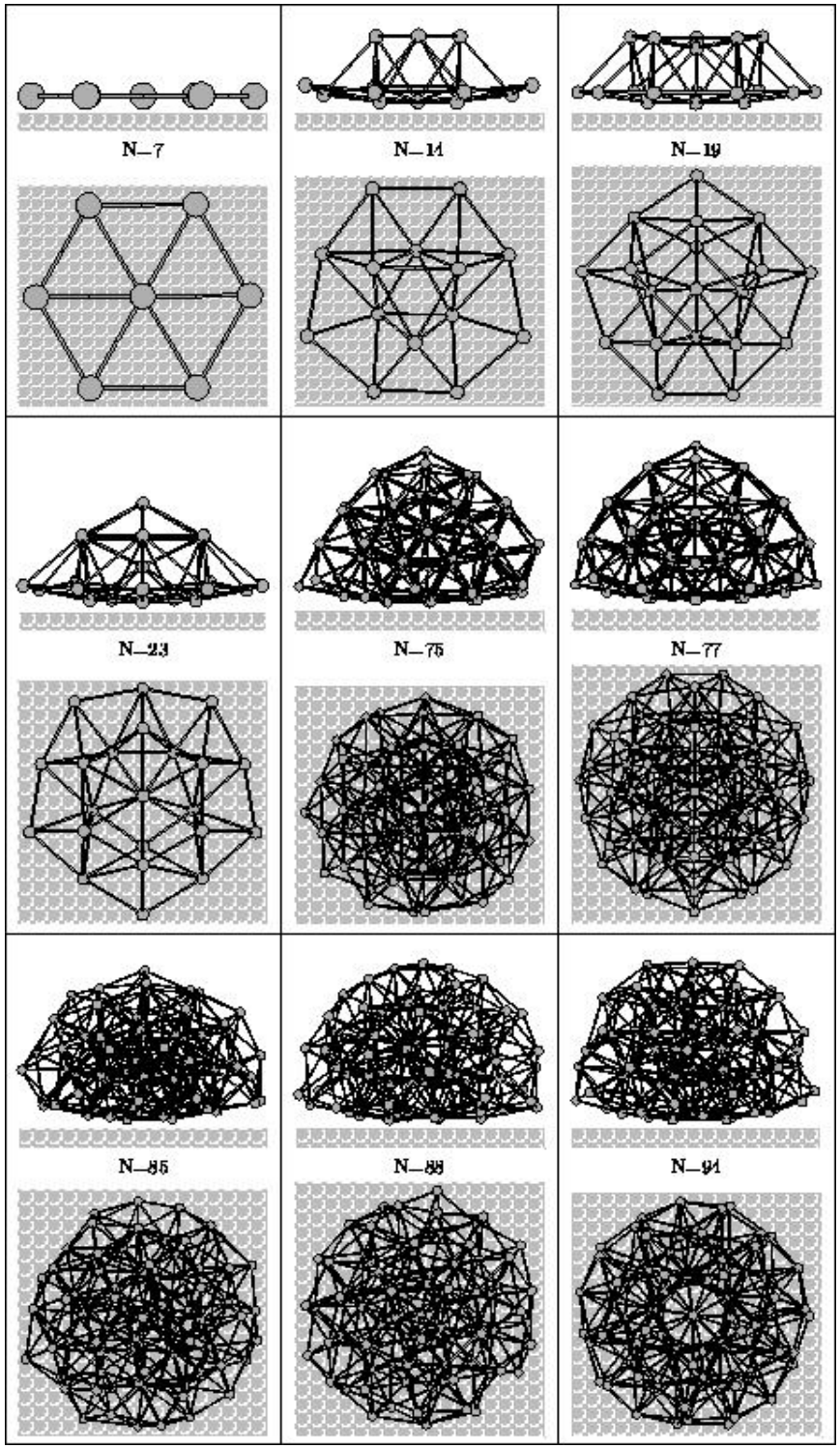
Minimization of $E_{pot}$

Quasi-classical energy $E_q = E_{kin} + E_{pot} - E_s$

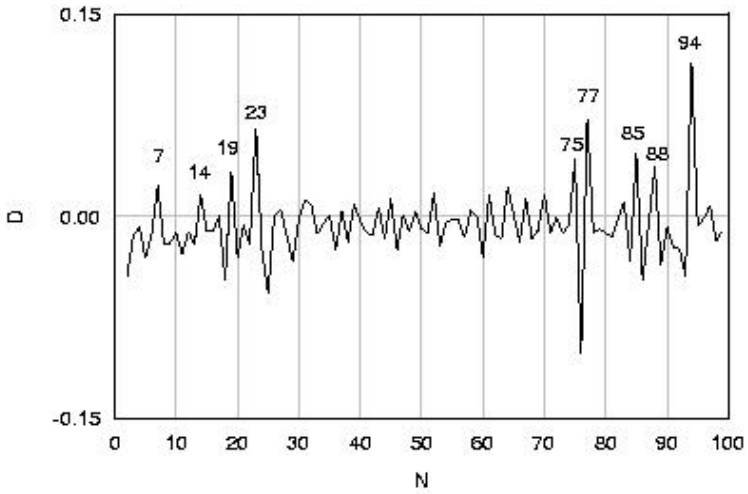
Binding energy $E = E_q + E_{ex}$

Interaction energy, breaking the cluster off the surface

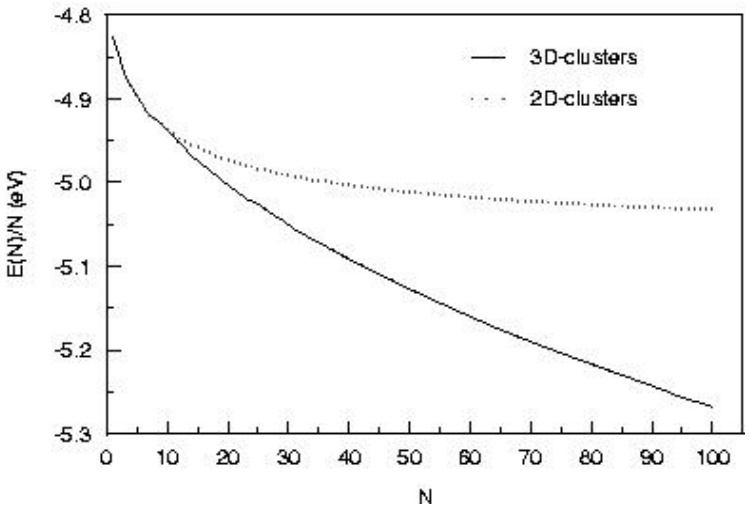
Diffusion, interfaces, more-or less-extended contacts

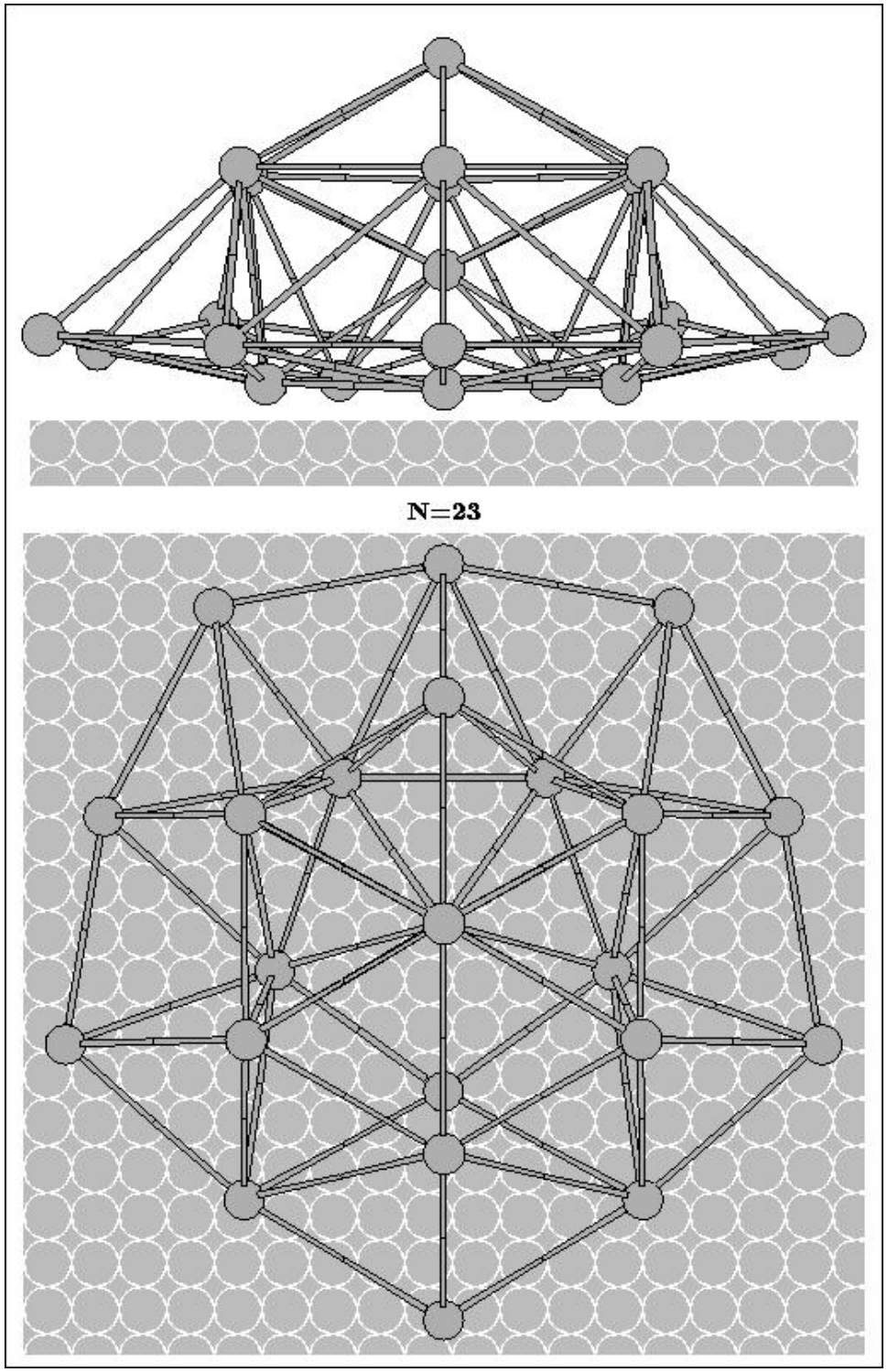

N–7
N–14
N–19
N–23
N–75
N–77
N–85
N–88
N–91

# Magic numbers

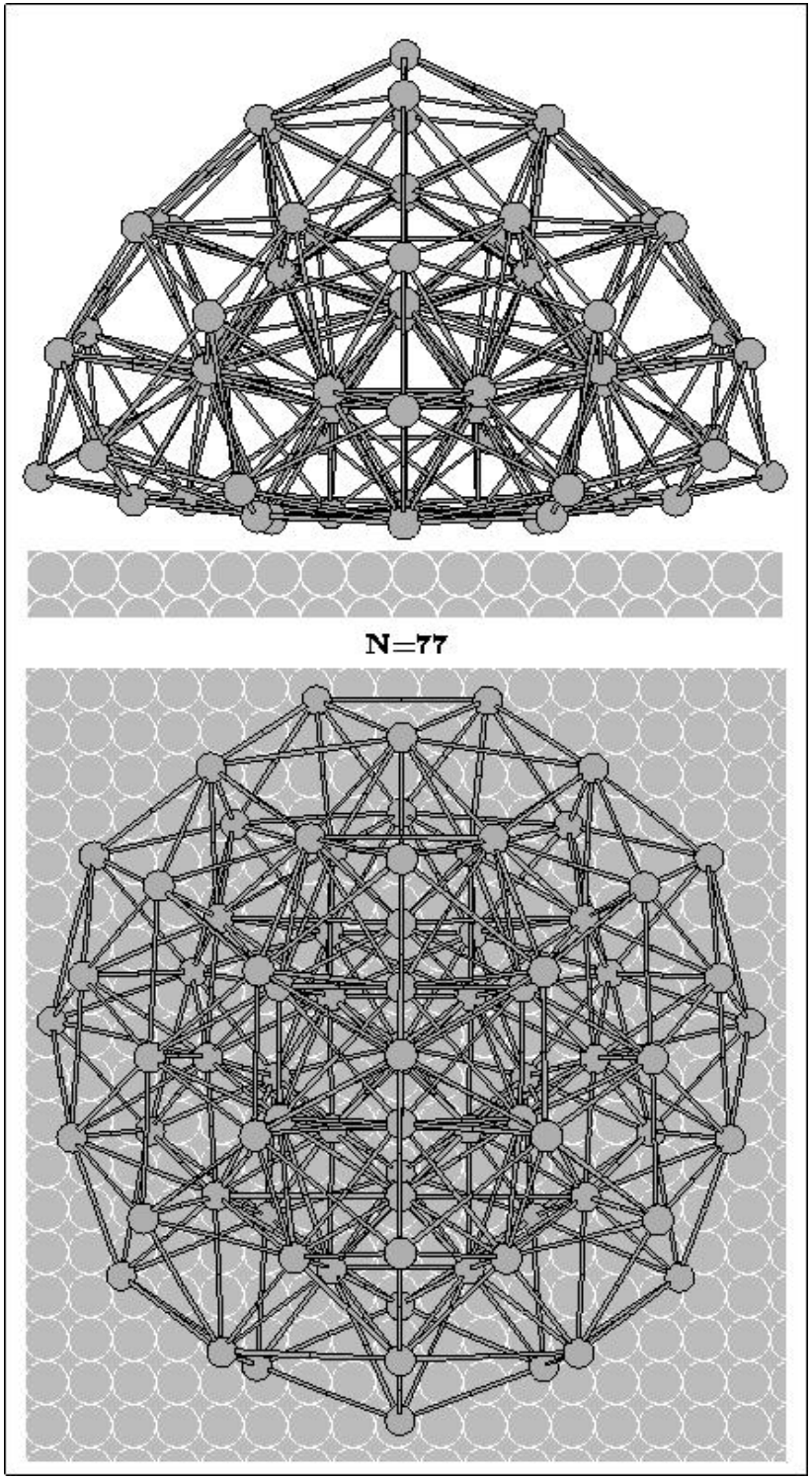



# Ground-state energy

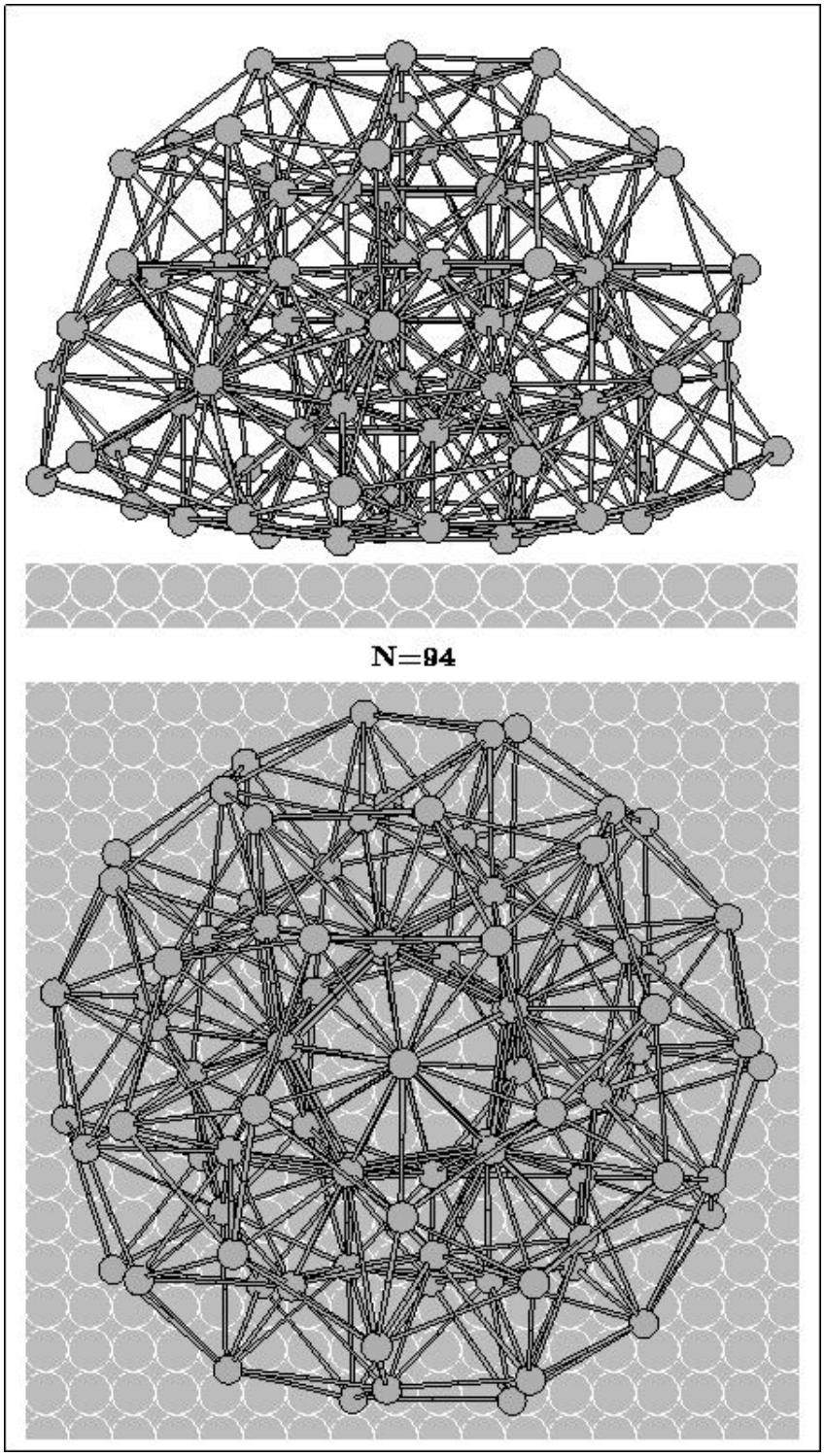


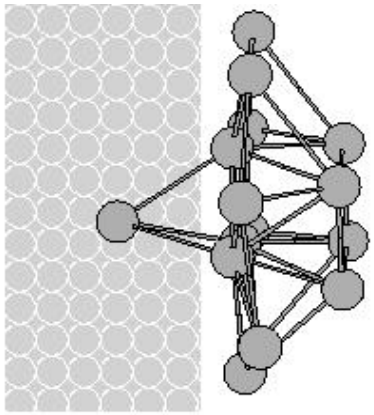


**N=23**

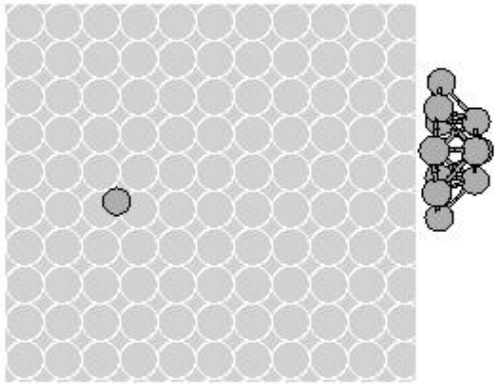


N=77

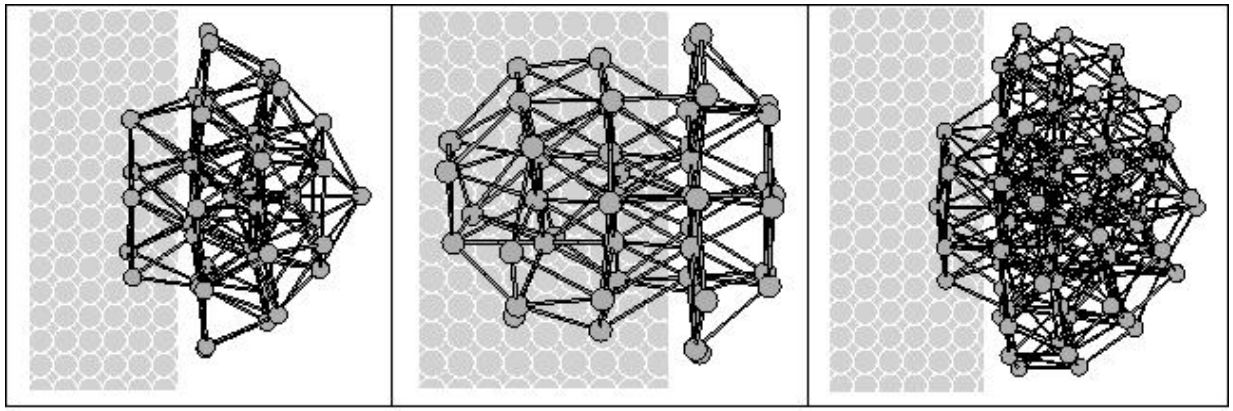

N=94



One atom beneath the surface



One atom escaped into solid



50-atoms cluster diffusing into solid,
100-atoms developing an interface with solid