Adsorption of the Superheavy Element Species on Gold Surface:

Relativistic Density Functional Study

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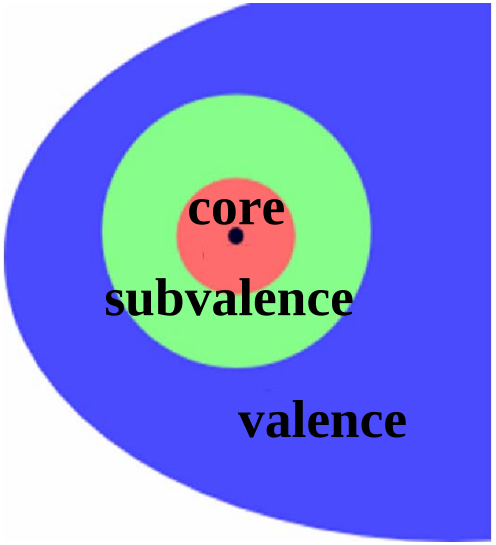
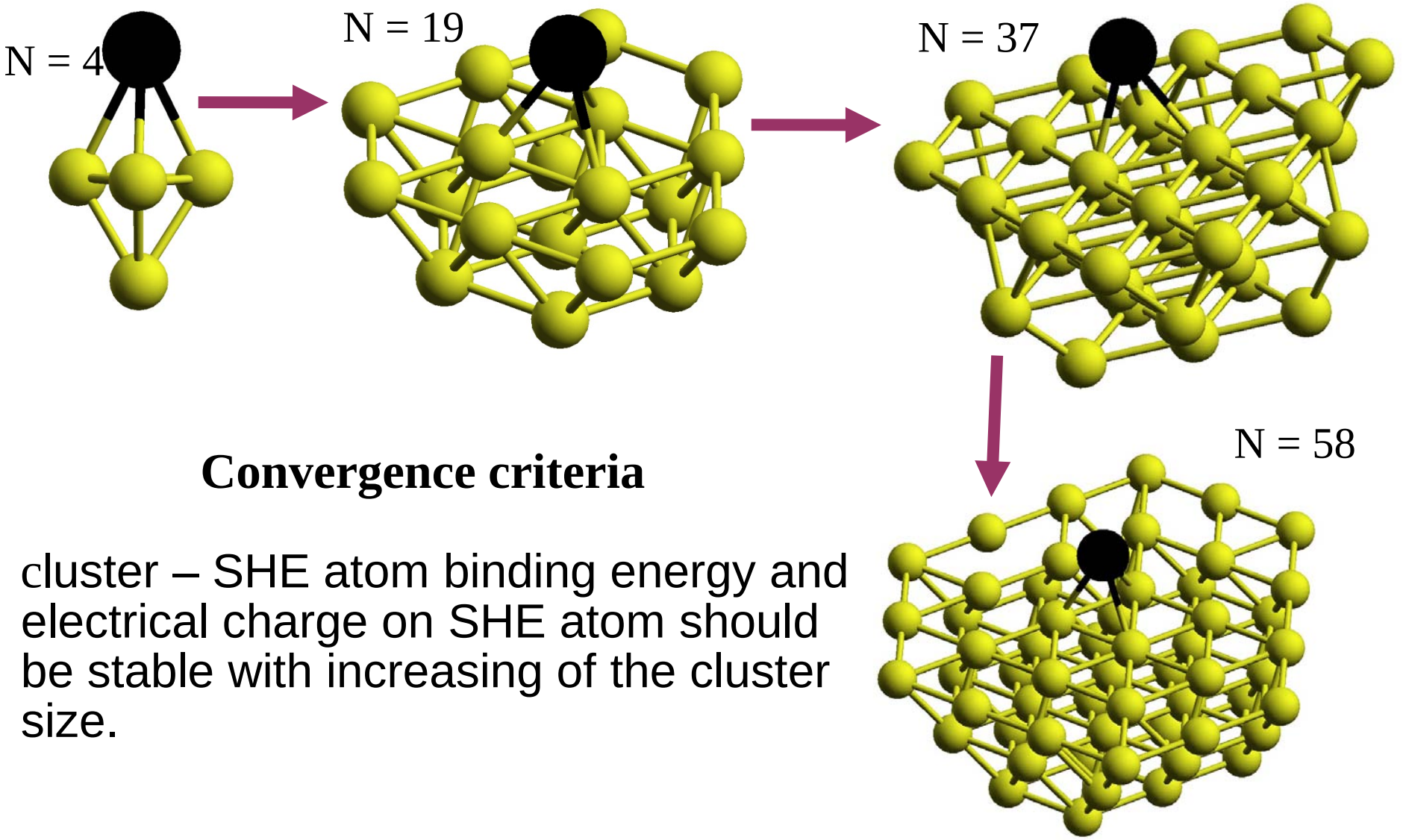
Computational details



- shape-consistent small-core pseudopotential approach;
- highly accurate relativistic theory methods of the electron structure for simplest molecular compounds;
- two-component relativistic density functional theory for sufficiently large systems.

Simulation of superheavy element atom adsorption

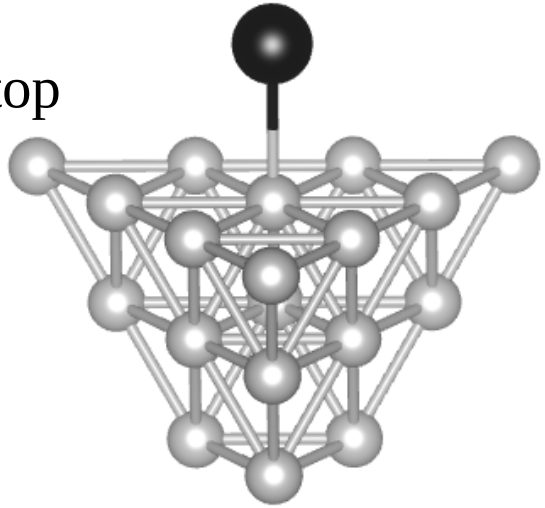


Convergence criteria

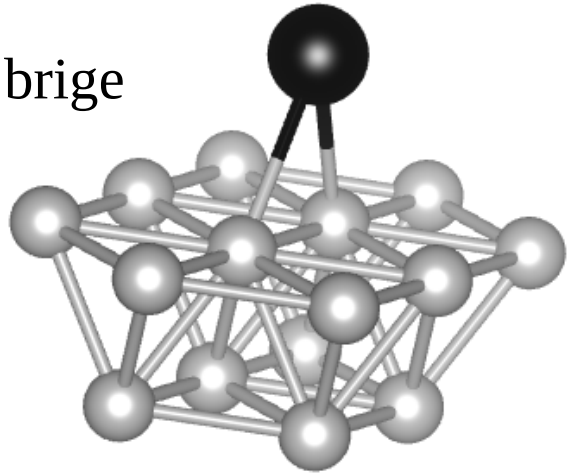
cluster – SHE atom binding energy and electrical charge on SHE atom should be stable with increasing of the cluster size.

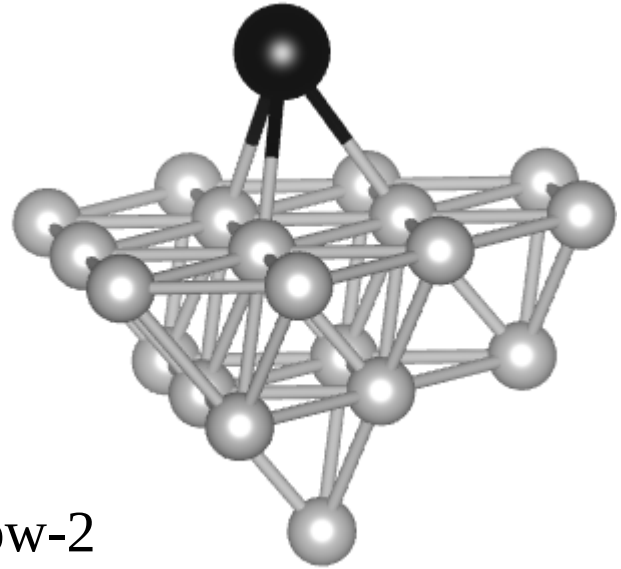
Energetically preferable adatom position under cluster

top

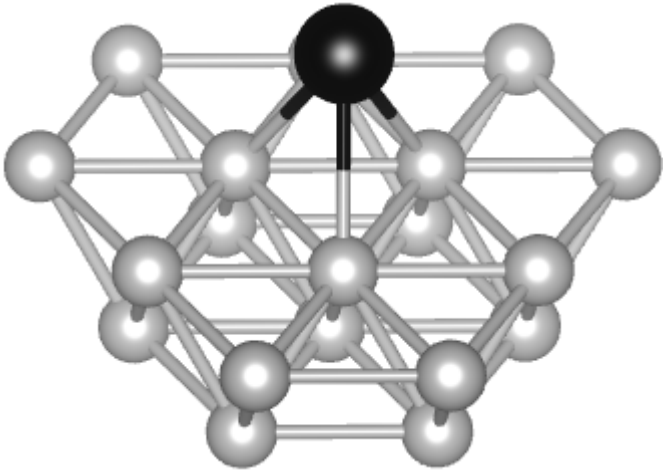


brige



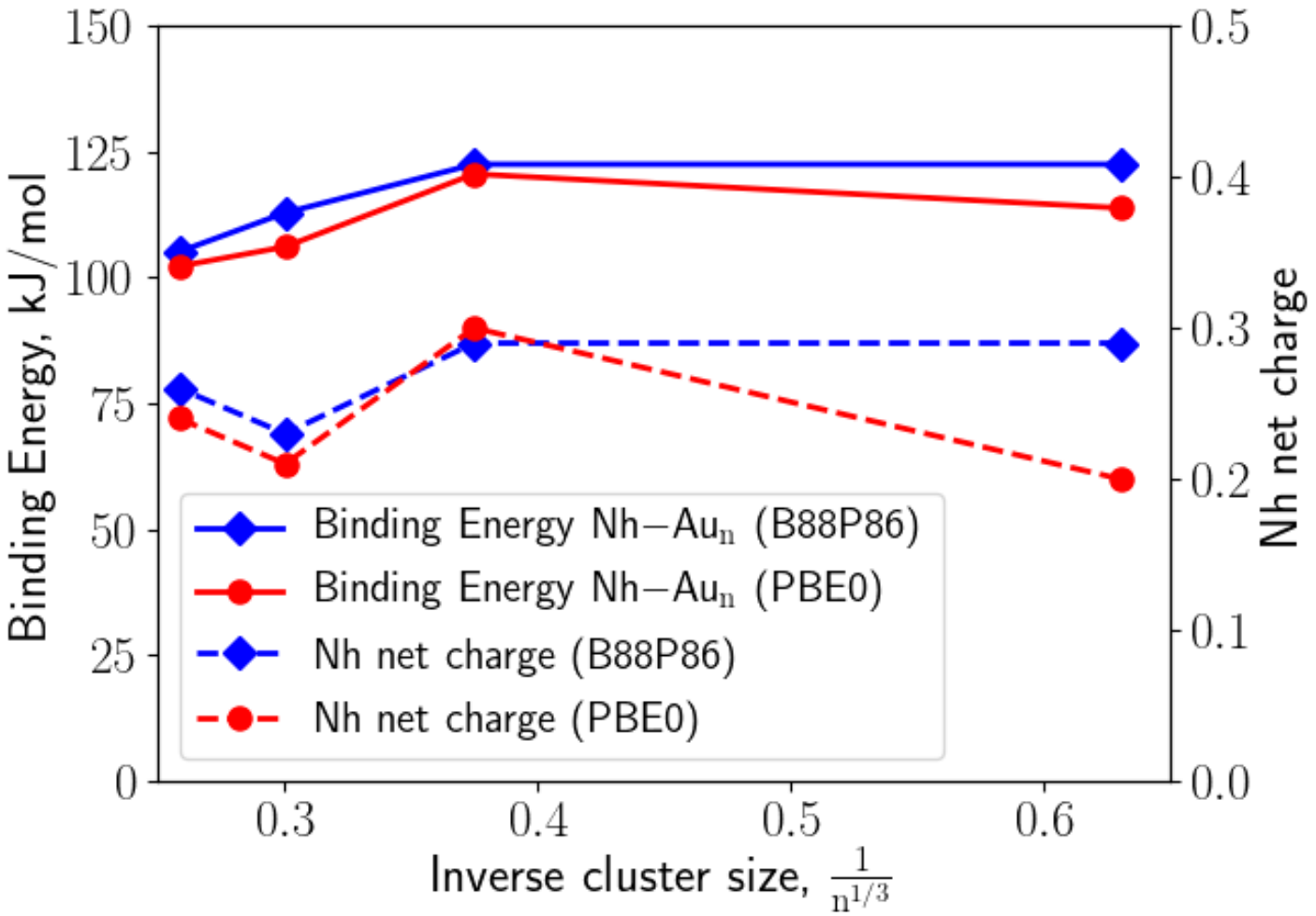


hollow-2



hollow-3

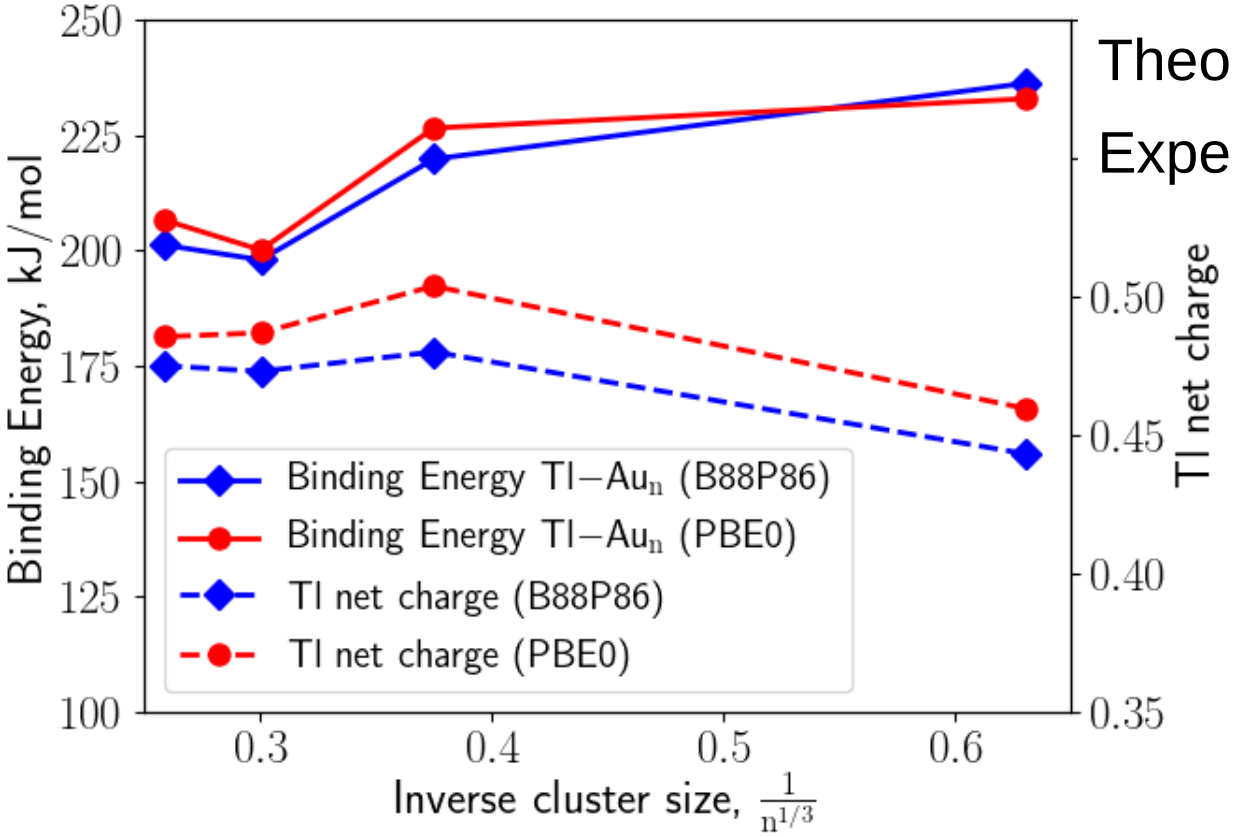
Nihonium *single atoms adsorption on gold surface*



Nh/gold adsorption energy estimates lie within the range **106 ± 10 kJ/mol**.
Experimental estimation for adsorption energy Tl/gold is **270 ± 10 kJ/mol**.

A.Rusakov, Yu. Demidov, A. Zaitsevskii Cent. Eur. J. Phys. (2013)

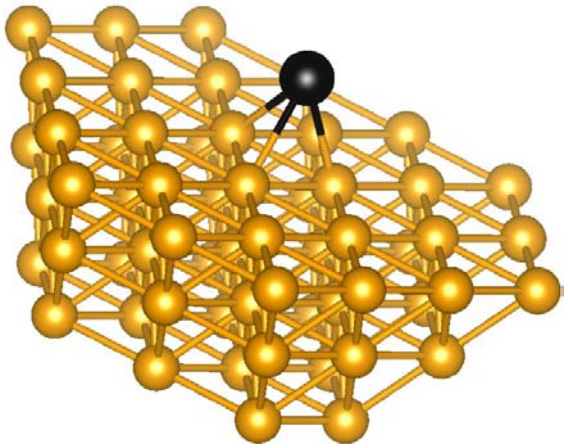
Thallium *single atoms adsorption on stable gold surface*



Tl/gold adsorption energy

Theory: **205 ± 10 kJ/mol**

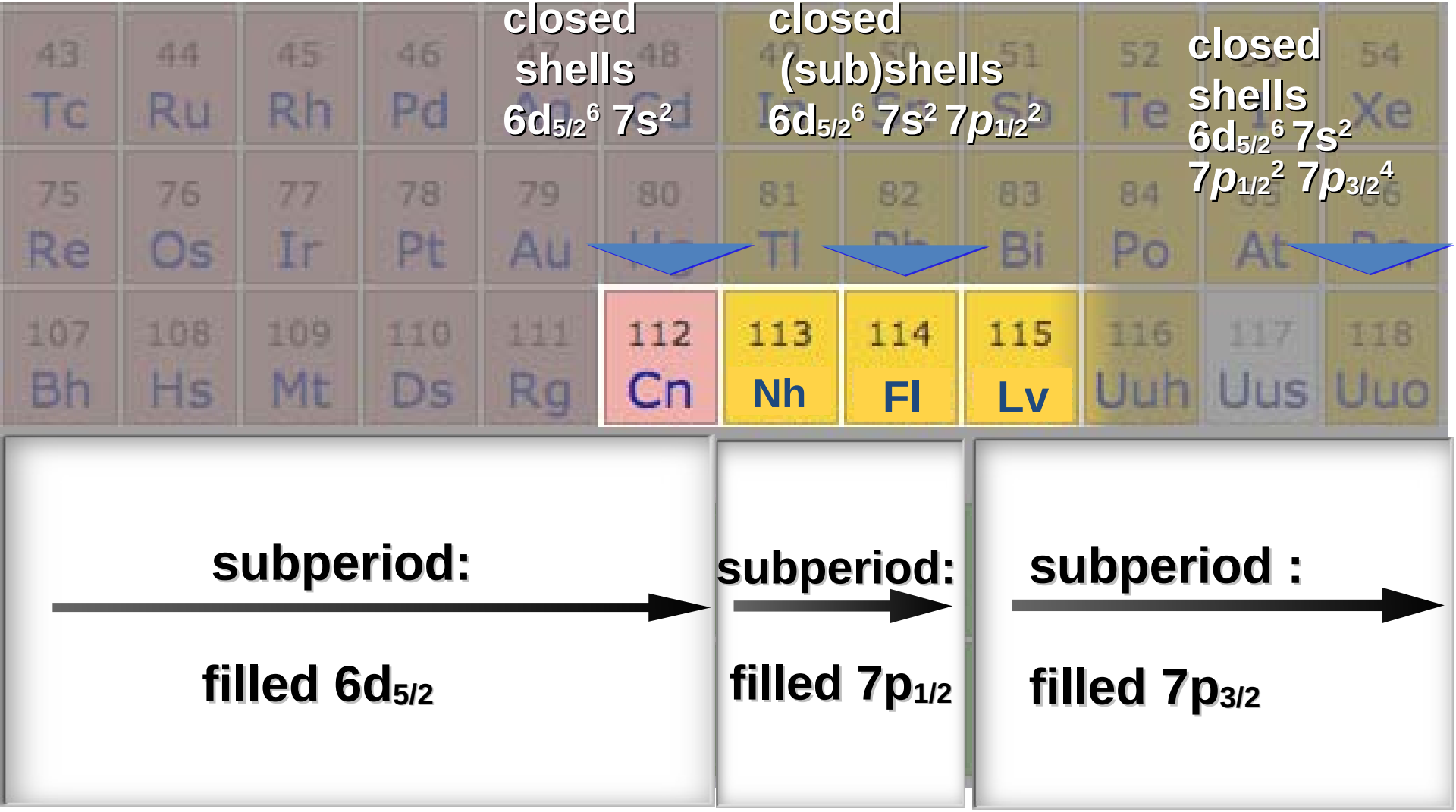
Experiment: **270 ± 10 kJ/mol**



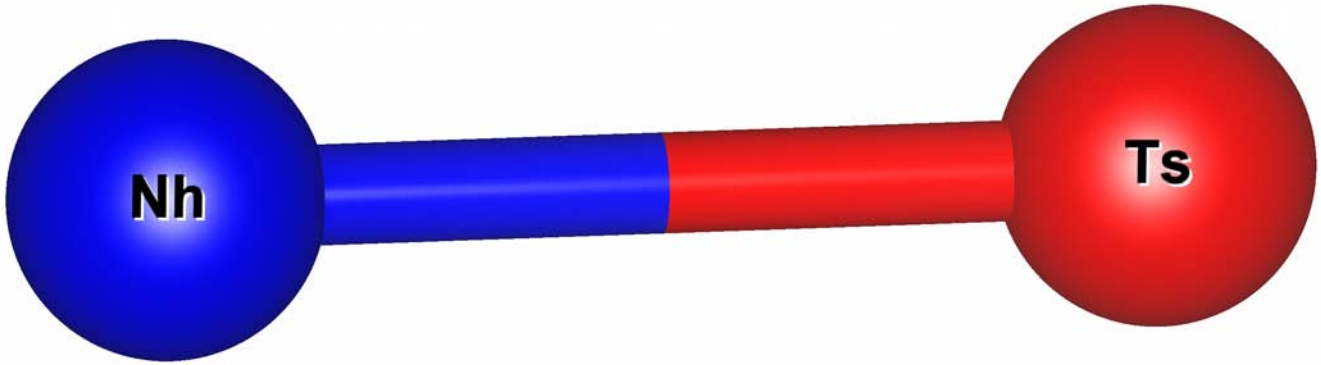
Difference between Nh and Tl atoms adsorption energies

Δ (DFT, present work)	99 ± 15 kJ/mol
Δ (DFT, van Wüllen, 2012)	90 ± 15 kJ/mol

7^{th} Period Subperiodic Structure



Bader charge distribution in NhTs *dimer*



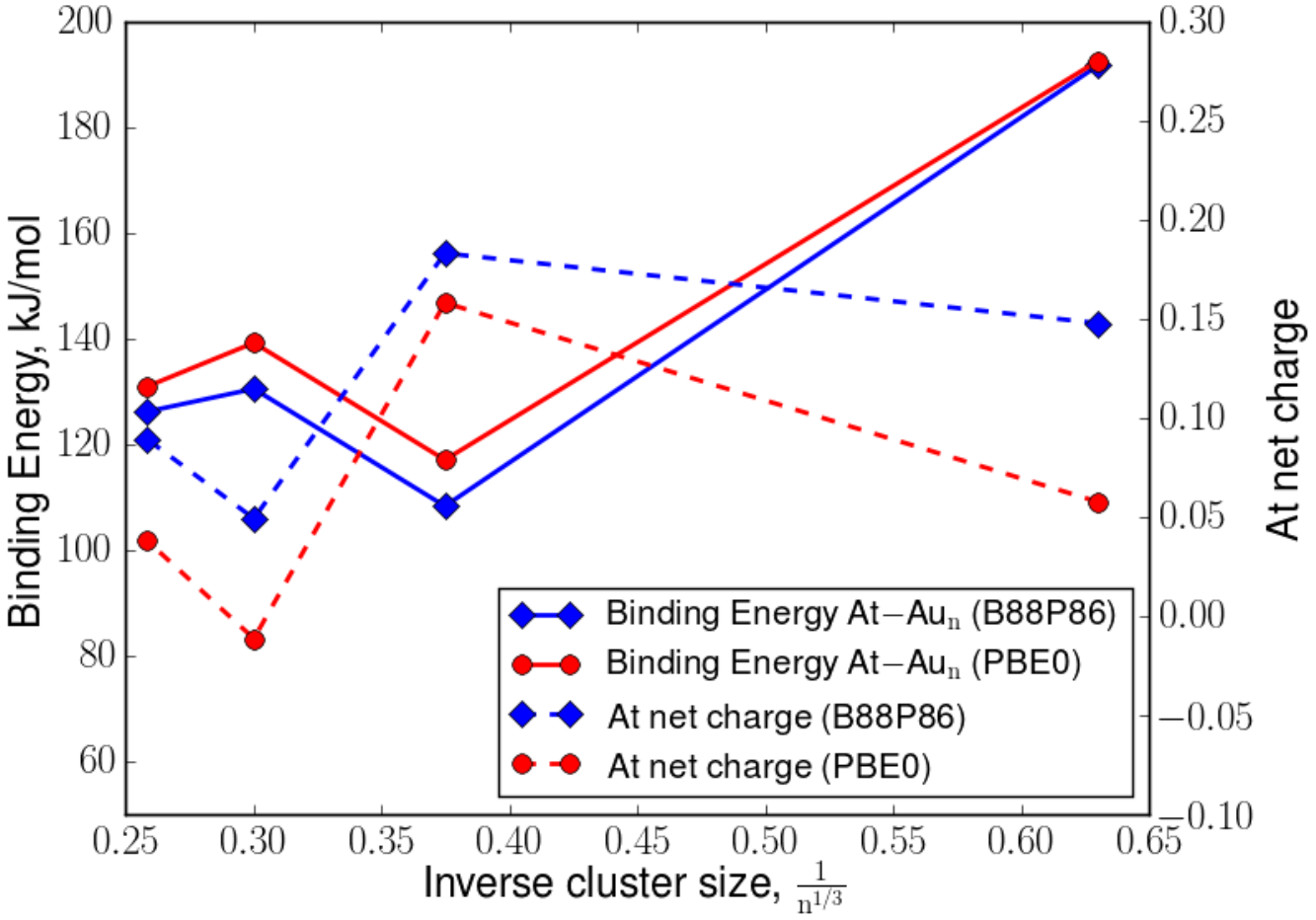
Including relativistic effects **Q = -0.056** **Q = +0.056**

Without relativistic effects **Q = +0.554** **Q = -0.554**

Cheolbeom Bae, et. al Chem. Phys. Lett. 37, 65 (2003)

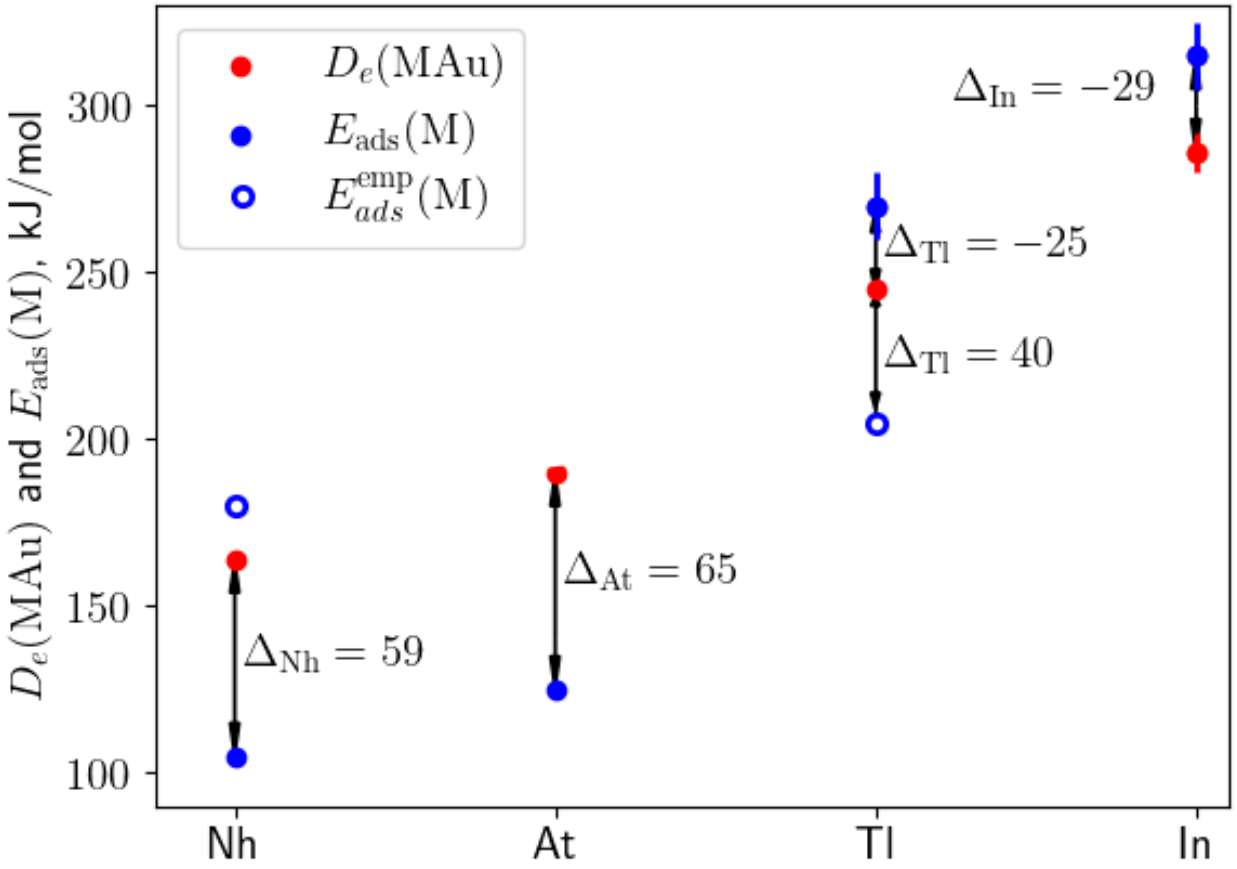
Which element is the most electronegative in 7th period?

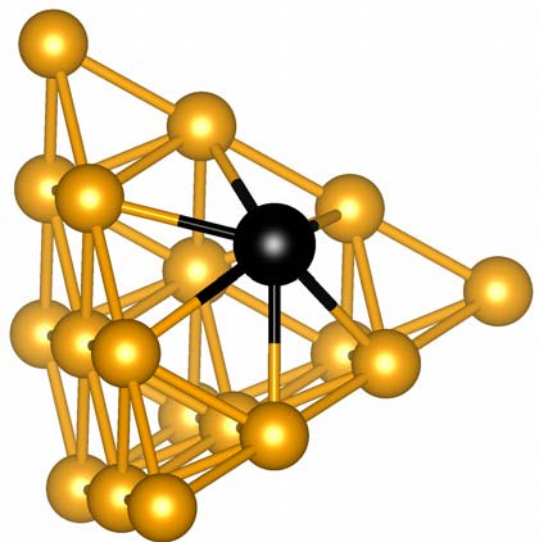
Astatine single atoms adsorption on gold surface



At/gold adsorption energy estimates lie within the range **130 ± 10 kJ/mol**.
Experimental estimation for adsorption energy At/gold is **147 ± 15 kJ/mol**.

Semiempirical regularities





M	Nh	At	Tl	In
ΔH_{LS} [kJ/mol]	66	28	-22	-62

Surface vacancy is formed, if partial molar solution enthalpy of the adsorbate M in the solid gold is negative.

Energy of surface vacancy formation for gold

Tl/gold adsorption energies

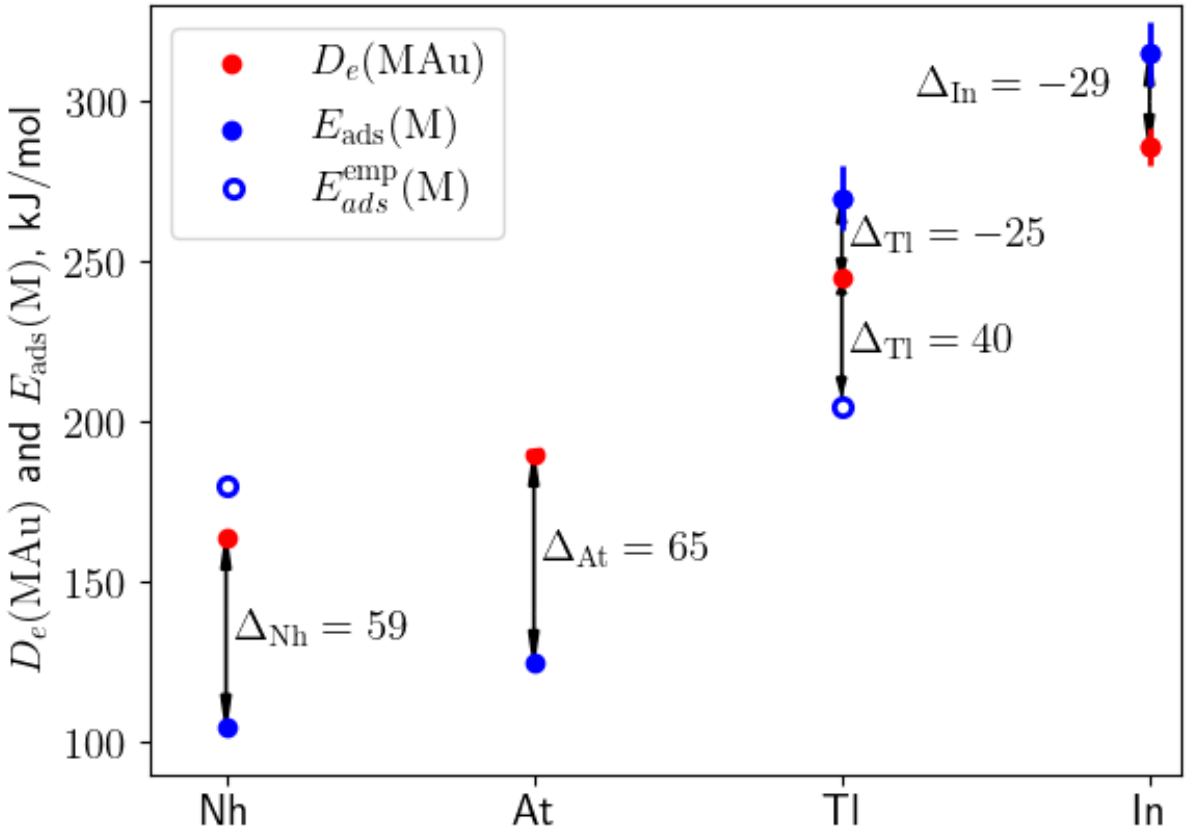
On stable surface: **205 ± 10 kJ/mol** (DFT)

In vacation position: **270 ± 10 kJ/mol** (Experimental)

Energy of surface vacancy formation for gold

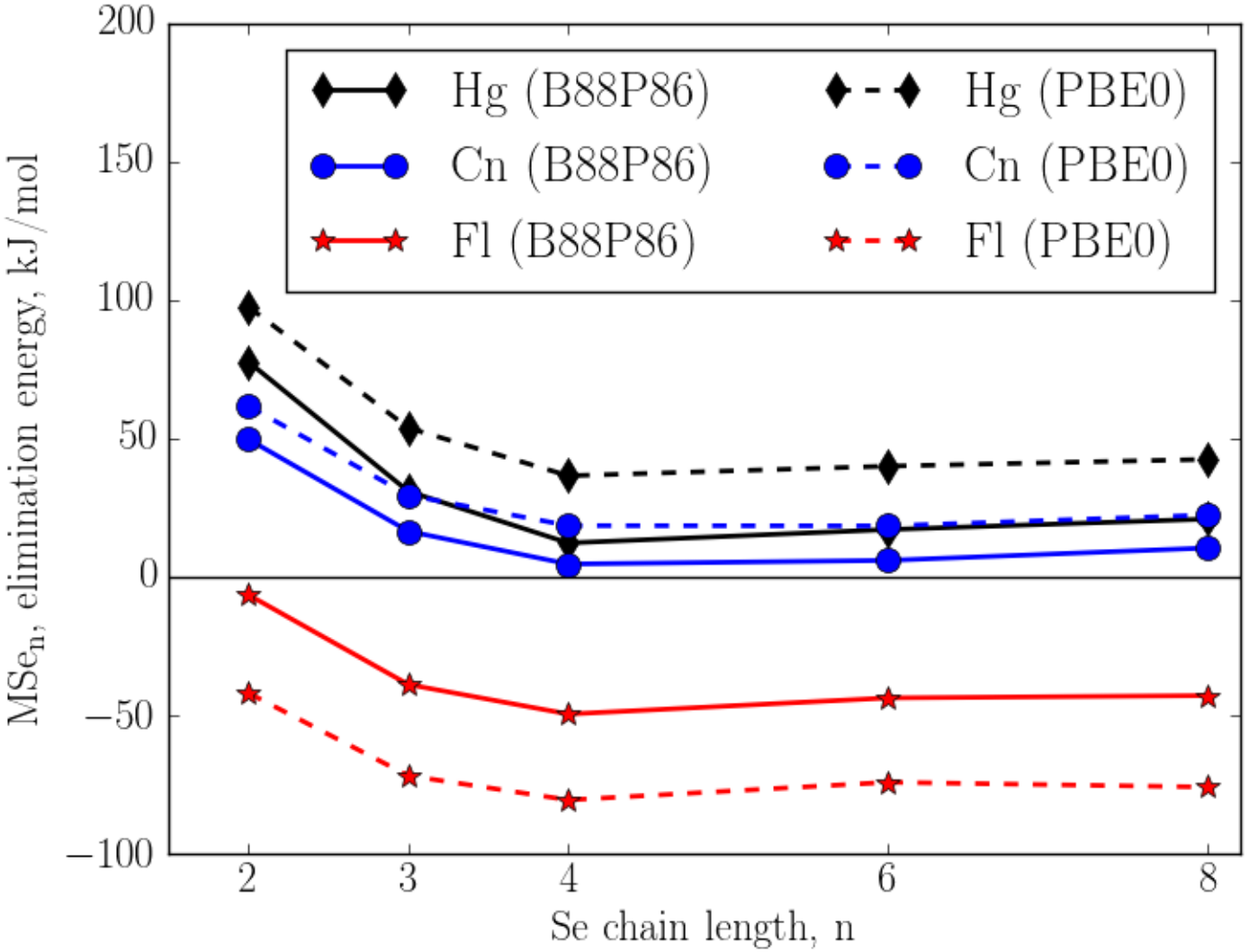
Semiempirical: **65 ± 15 kJ/mol**

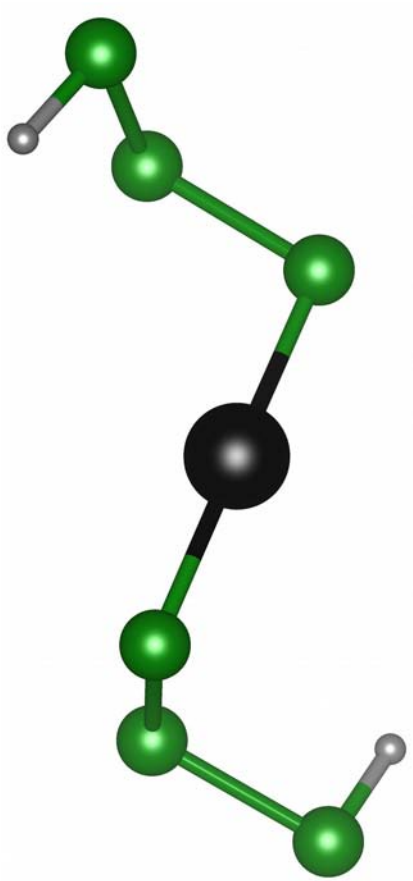
Experimental: **77.19 kJ/mol**



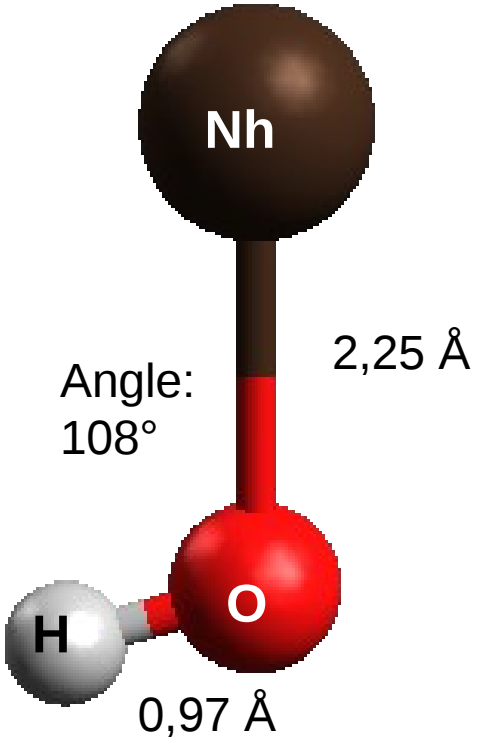
Hg, Cn, Fl *atoms adsorption on red selenium surface*

PRELIMINARY

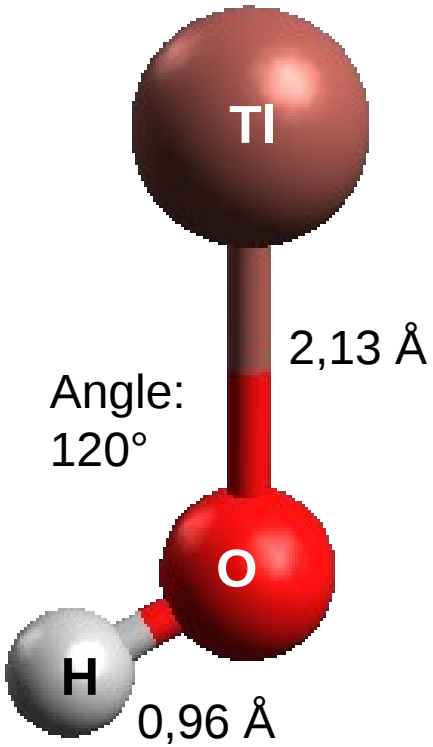




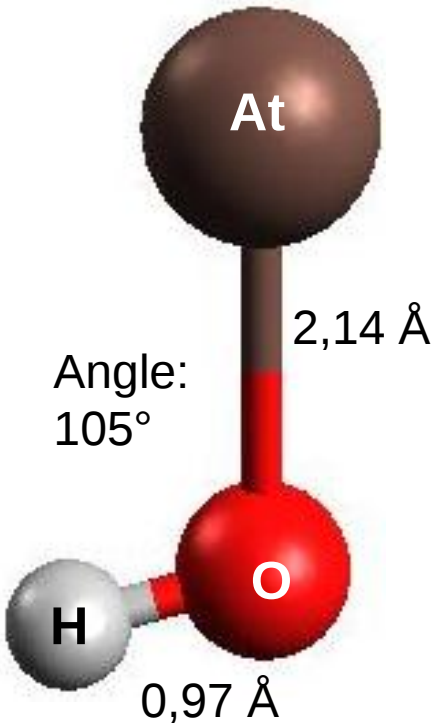
Structure and properties of NhOH, AtOH *and* TlOH



D_0 (Nh-OH)
2.02 eV



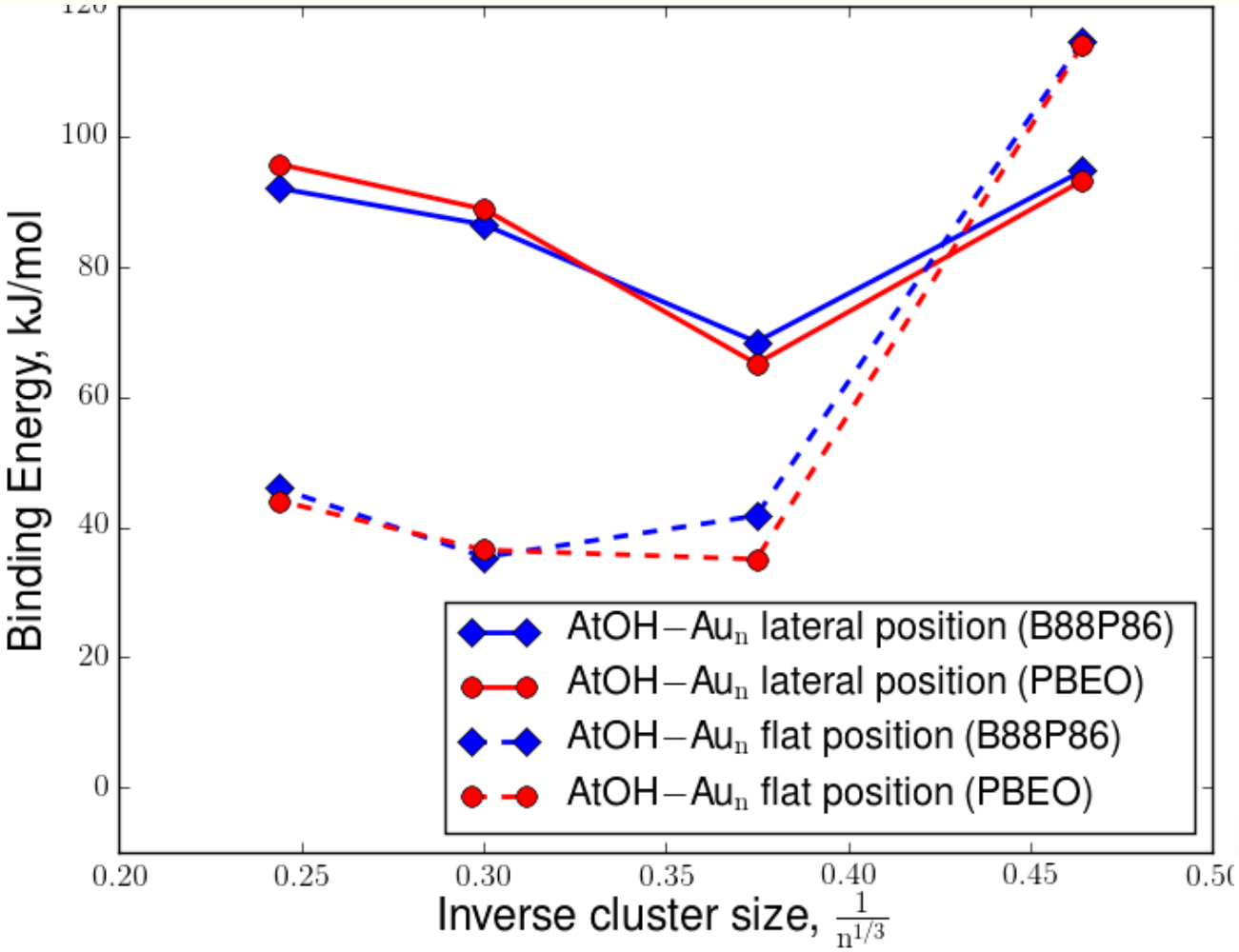
D_0 (Tl-OH)
3.34 eV

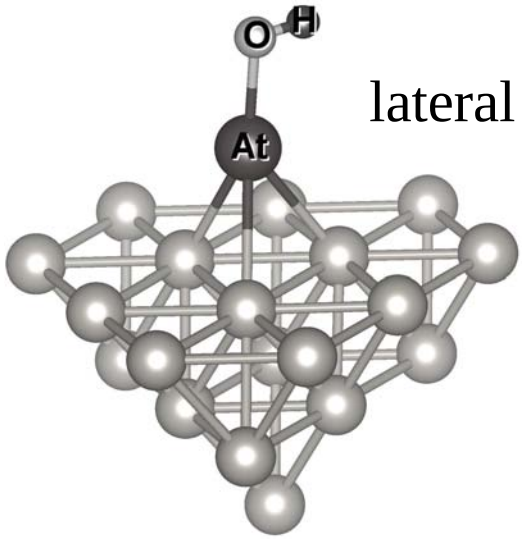


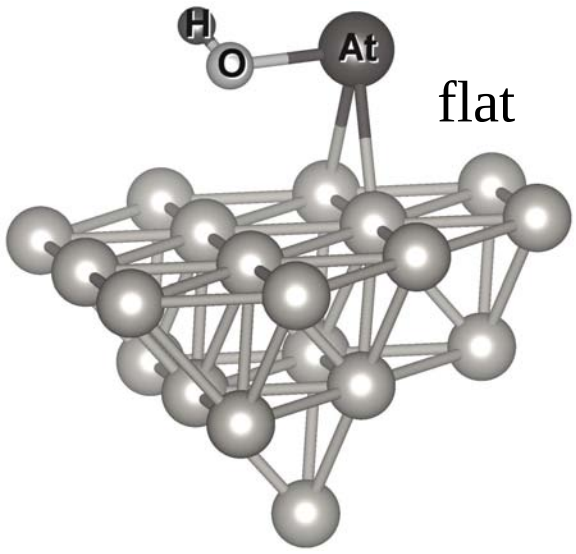
D_0 (At-OH)
1.89 eV

Yu.Demidov, A. Zaitsevskii Chem. Phys. Lett, 638, 21 (2015)

AtOH *adsorption on gold surface*







AtOH/gold adsorption energy

Theory: **90 ± 10 kJ/mol**.

Experiment: **100 +20/-10 kJ/mol**.

Thank you for attention!