Predictions of Adsorption of Elements 112 and 114 on Various Surfaces

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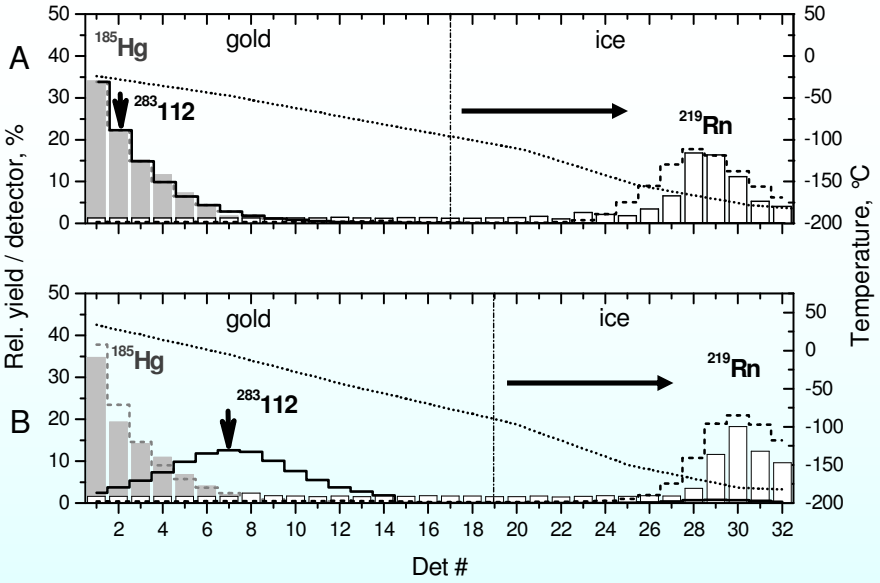
Experimental Observations



112

114

T_{ads}(exp.) = -5 °C

ΔH_{ads}(exp.) = -52_{-4}^{+20} kJ/mol

T_{ads} = -88 °C

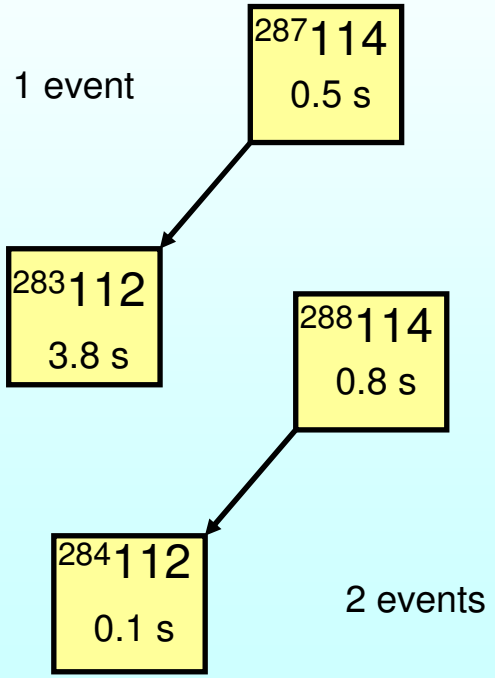
ΔH_{ads} = $-35\ ^{+19}_{-3}$ kJ/mol

112: R. Eichler, *et al*. Nature, **447**, 72 (2007)

114: Science News Online, April, 12, 2008;

Vol. 173, Nr. 15

R. Eichler, *et al*. NRC7, Budapest, 2008, Abstract



Atomic Properties of Elements 112 and 114 and Adsorption on Inert Surfaces

$$E(x) = -\frac{3}{16}\left(\frac{\varepsilon - 1}{\varepsilon + 2}\right)\frac{\alpha_{mol}}{\left(\frac{1}{IP_{slab}} + \frac{1}{IP_{at}}\right)R_{vdW}^{\ 3}}$$

DCB CCSD(T) calculations (A. Borschevsky)

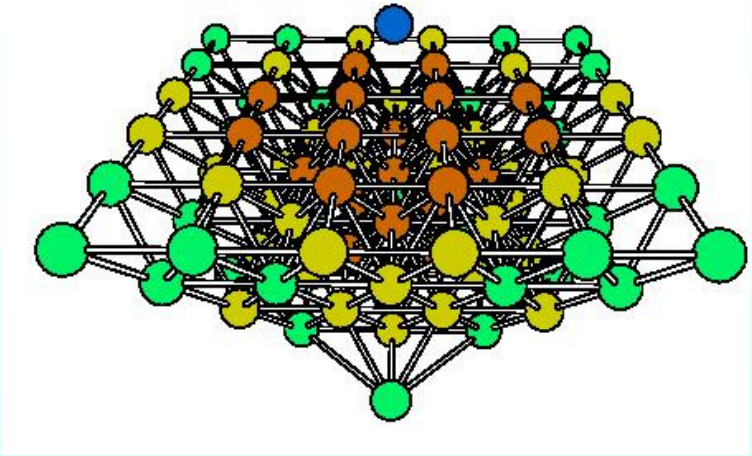
Property	112	114
Electronic configuration	$d^{10}s^2$	$s^2p_{1/2}^{\ 2}$
IP, eV	11.97	8.54
α, a.u.	27.4	29.5
AR, a.u.	3.21	3.30
R_{vdW}, a.u.	3.75	3.94
ΔH_{ads}(quartz), kJ/mol	27	21
ΔH_{ads}(ice), kJ/mol	26.2	20.2
ΔH_{ads}(Teflon), kJ/mol	16.4	10.4

V. Pershina *et al*. J. Chem. Phys. 128, 024707 (2008)

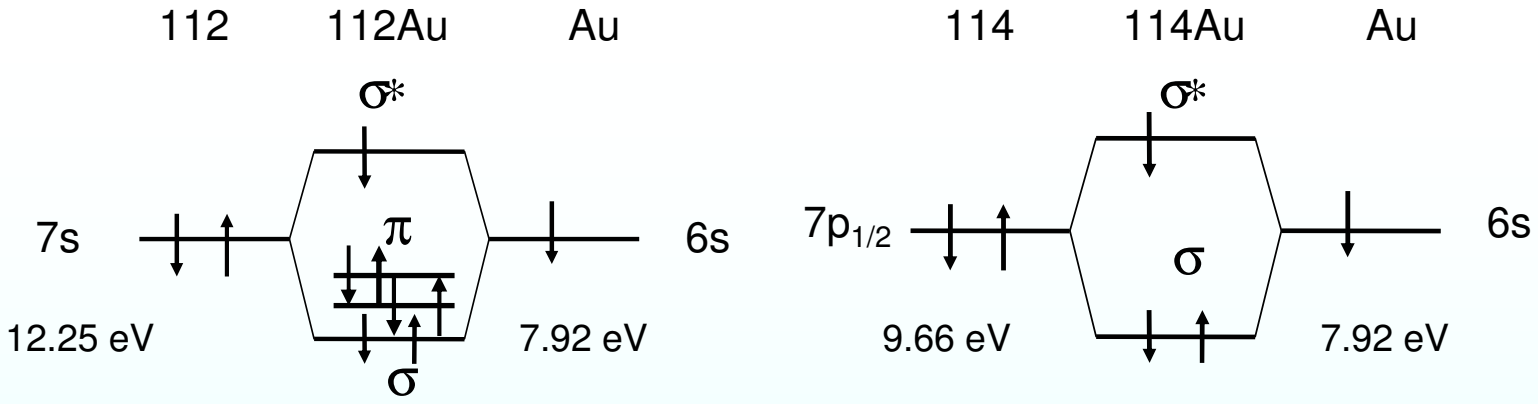
Predictions of Interaction of Elements Hg/112 and Pb/114 with Metals

4*c* - DFT calculations for:

- dimers MAu (V.P.)
- medium-size and large clusters MAu_n (J. Anton)
  - n=16 ... n=120
- embedded clusters $(MAu_n)Au_m$
  - n=34-36 m=156



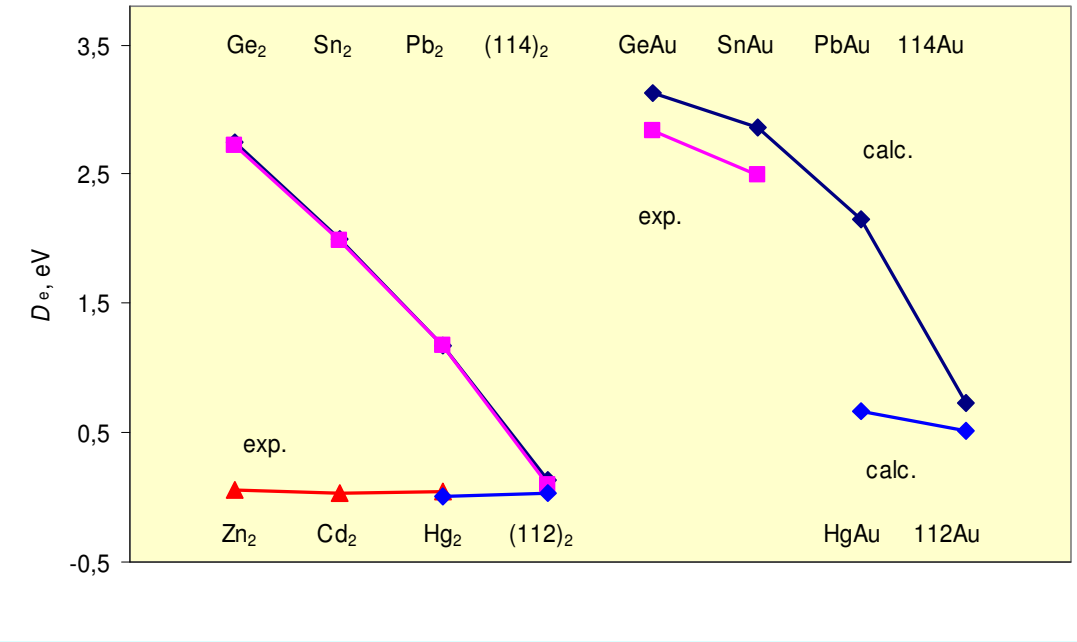
MO Energies and Composition of 112Au and 114Au

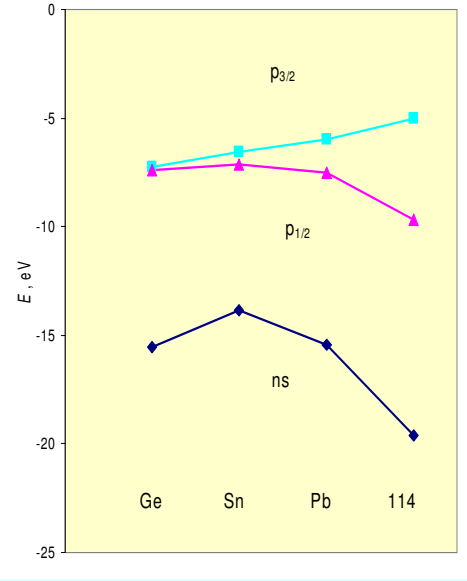


112Au			114Au		
MO	Energy, eV	Composition, %	MO	Energy, eV	Composition, %
σ_{112}	-3.007	(68)$7p_{1/2}$(**112**)+(11)6s(Au)+(8)$6p_{3/2}$(Au)	π_{114}	-2.34	(94)$7p_{3/2}$(**114**)+(2)$5d_{5/2}$(Au)+(3)$6p_{3/2}$(Au)
σ_{Au}*	-5.885	(11)7s(**112**)+(72)6s(Au)+(9)$5d_{5/2}$(Au)	σ_{114}*	-4.935	(39)$7p_{1/2}$(**114**)+(41)6s(Au)+(9)$5d_{5/2}$(Au)
π_{Au}	-6.542	(2)$6d_{5/2}$(**112**) +(98)$5d_{5/2}$(Au)	σ_{Au}	-5.797	(9)$7p_{1/2}$(**114**)+(30)6s(Au)+(57)$5d_{5/2}$(Au)
π_{Au}	-6.651	(16)$6d_{5/2}$(**112**)+ (84)$5d_{5/2}$(Au)	π_{Au}	-5.880	(100)$5d_{5/2}$(Au)
σ_{Au}	-6.756	(1.2)7s(**112**)+(4)$6d_{5/2}$(**112**) + (87)$5d_{5/2}$(Au)+(4)6s(Au)	π_{Au}	-6.123	(0.7)$7p_{3/2}$(**114**)+(98)$5d_{5/2}$(Au)+(0.5)$5d_{3/2}$(Au)
Ground	$^2\Sigma^+$	$d_{Au}^{10}\sigma_{Au}^{2}\sigma^{*}_{Au}{}^{1}$	Ground	$^2\Sigma$	$d_{Au}^{10}\sigma_{Au}^{2}\sigma^{*}_{114}{}^{1}$

* HOMO

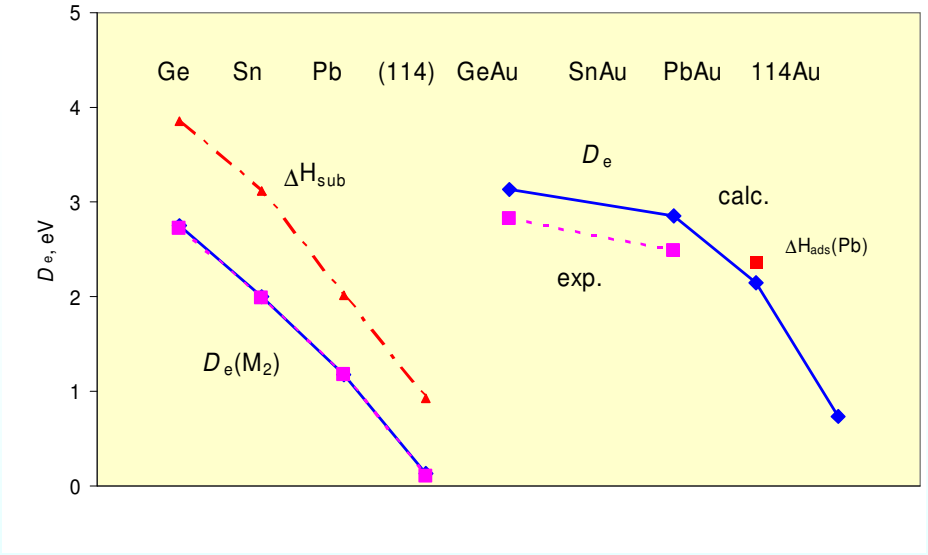
Comparison of Group 12 and 14 Dimers

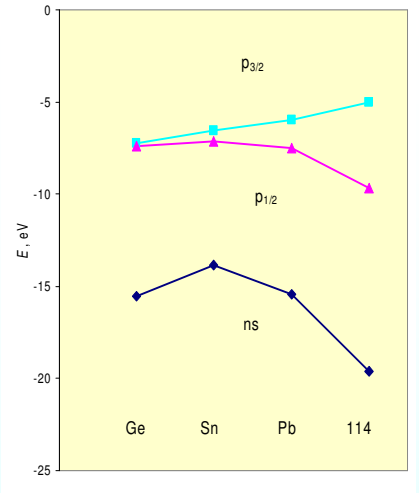




Element 114 should be more reactive than 112. Large difference between Pb and element 114.

Correlation between $D_e(M_2)$ and $\Delta H_{sub}/\Delta H_{ads}$

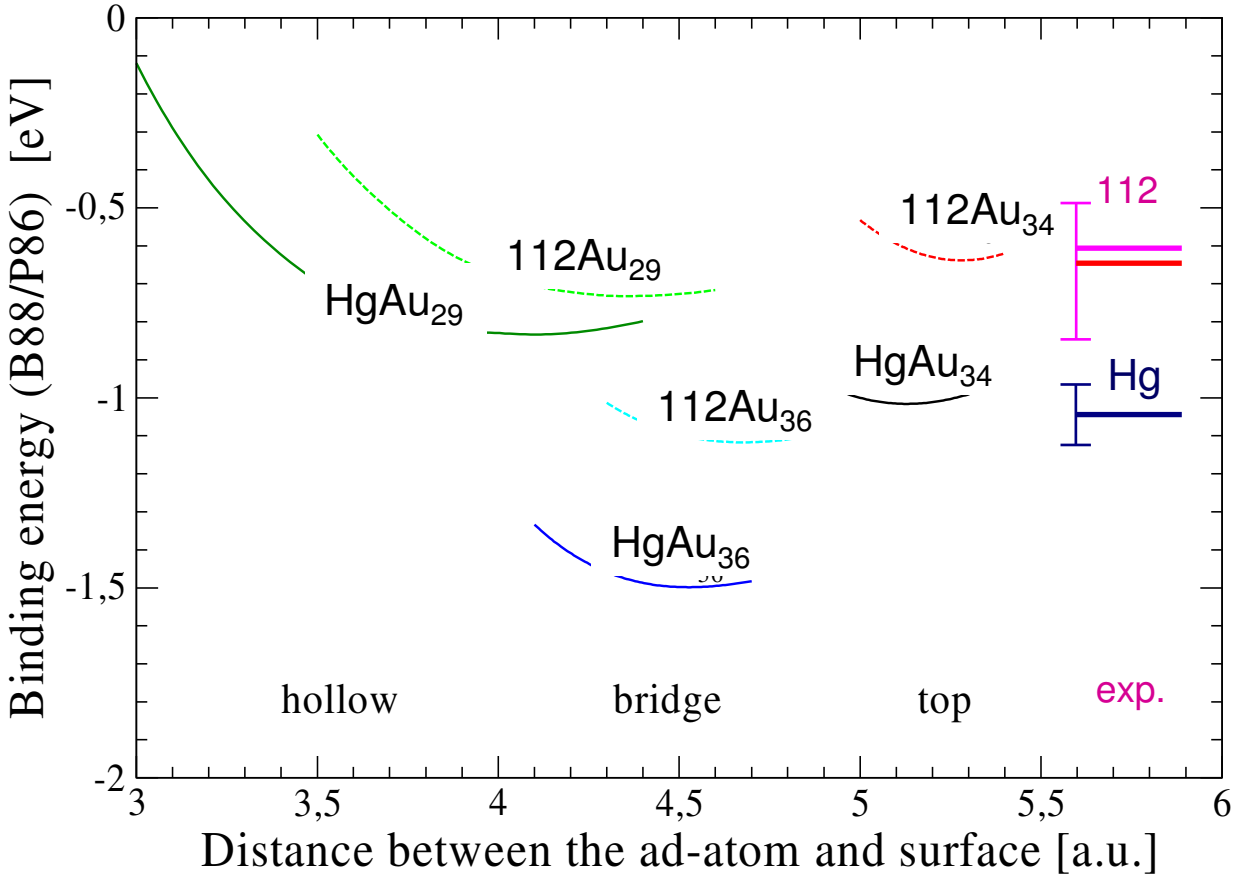




Molecule	D_e, eV	ΔH_{ads}, eV	Molecule	D_e, eV	ΔH_{ads}, eV
Ge_2	2.70	1.76	GeAu	3.14	-
Sn_2	2.00	1.18	SnAu	2.86	-
Pb_2	1.17	2.02	PbAu	2.15	2.37
$(114)_2$	0.13	0.93	114Au	0.73	(0.95)
		0.74±0.16*			(0.97)*

* H. Rossbach and B. Eichler

Results of Embedded Cluster Calculations



112

Predicted:

T_{ads}(calc.) = 0 ℃

ΔH_{ads}(calc.) = - 62 kJ/mol

[V. Pershina *et al.*, Nucl. Phys. A **734**, 200 (2004); *ibid* **787**, 381 (2007)]

Observed:

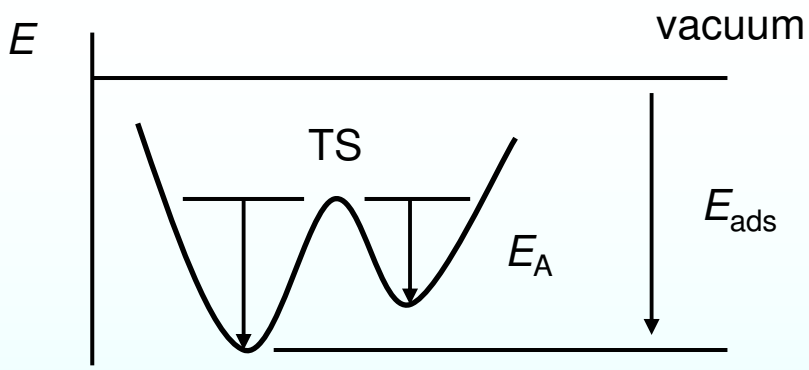
T_{ads}(exp.) = -5 ℃

ΔH_{ads}(exp.) = -52_{-4}^{+20} kJ/mol

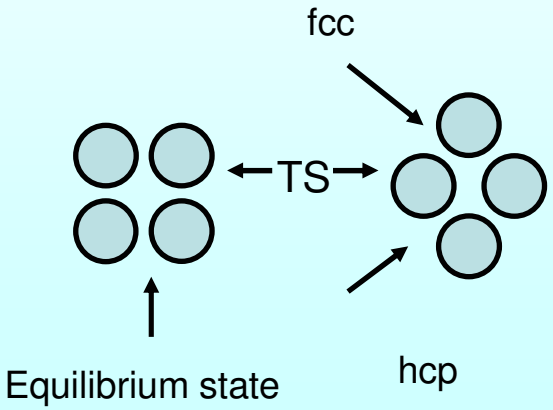
[R. Eichler, *et al.* Nature, **447**, 72 (2007)]

C. Sarpe-Tudoran *et al.* J. Chem. Phys. **126**, 174702 (2007)]

Comparison of Au(100) and Au(111) Surfaces



(100) (111)



Surface reconstruction

Au(100) face-centered-cubic (fcc)

hexagonal-close-packed (hcp)

Surface	E_A, eV
Au(100)	0.62
Au(111)	0.22
Δ	0.40