

## Electron Affinity Of Metals And Strain

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**Abstract:** In the present paper we theoretically review the dependence of electron affinity of metals on electron density profile and strain using electron approximation theory. Result obtained revealed that electron affinity of metals increases as the electron density parameter increases. This increase may be due to change in atomic radius, nuclear charge and electronic configuration of electrons in the metals. The result obtained for electron affinity in this work is negative. This can be due to the fact that electron affinity is the energy released when electron binds to an atom and can also be due to the fact that electron affinity is the quantitative measurement of energy change that results from adding a new electron to a neutral atom. There is a good agreement between the computed and ab-initio value of electron affinity of metals. In this work, electron affinity of metals rises as strain increases. This increase is caused by change in band structure and energy levels of electrons in the metals. The increase in the electron affinity of metals as strain increases could be due to the contact energy barrier between the electrons in metals that reduces as the strain increases.

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### Introduction

Metals are characterized by high electrical conductivity. Metals possess large number of electrons that are free to move about Kakani and Kakani (2004). The electrons that move about in metals are the conduction electrons Efthimios (2003). The valence electrons of atom become conduction electrons of metal. Metals tend to crystallize in relatively close packed structures: hcp, fcc, bcc, and some other closely related structures, and not in loosely-packed structures such as diamond Ashcroft and Mermin (1976). In transition metals there is additional binding from inner electron shells Elliott (1997). Transition metals and metals following them in periodic table have large d-electron shells and are characterized by high binding energy Pillai (2010). We can understand many physical properties of metals, and not only of the simple metals, in terms of the free electron model Efthimios (2003). According to this model, the valence electrons of the constituent atoms become conduction electrons and move about freely through the volume of metal Kachhava (1992). The utility of the free electron model is greatest for properties that depend essentially on kinetic properties of conduction electrons Rogalski and Palmer (2000). Metals usually form closed packed fcc, bcc, or hcp structures where electrons are shared by all the atoms Busch and Schade (1976). Metallic bonding energy is determined by a balance between the negative energy of Coulomb

interaction of electrons, positive ions and positive kinetic energy of electron Fermi gas Rogalski and Palmer (2000). Electron affinity is the change in energy of neutral atom in gaseous phase when electron is added to atom to form negative ion Ashcroft and Mermin (1976). The electron affinity is the energy change that occurs when an atom gains electron and releasing energy in the process Elliott (1997). Electron affinity is the energy released when an electron is added to a gaseous atom which is in its ground state to form a gaseous negative ion termed as first electron affinity Efthimios (2003). The smaller the first electron affinity, the easier an atom gains electrons Animalu (1977). The greater the electron affinity, the weaker is the ability of an atom to gain electrons. Ionization energy shows the ability of an atom to lose its electrons Kittel (1976). The electron theory of metals describes how electrons are responsible for the bonding of metals and subsequent physical, chemical and transport properties Animalu (1977). Before now, different theoretical model has been developed and used to study different properties of metals. Adesakin et. al (2023) develop a general formulation for coherence length of electron in metal based on Heisenberg approximation using free electron theory. This study was carried out to evaluate the behaviour of coherence length of electron under strain and electron density parameter. The result obtained agree quite well with theoretically obtained experimental value. There

is high concentration of electron coherence length in the region of high density limit than the low density limit. The high electronic concentration of electron coherence length in metals in the region of high density limit is due to an increase in Fermi surface of metals in the region. The electron coherence length of metal increases as the electron density parameter increases. These suggest that the electron coherence length of metal relied on the cohesive and repulsive forces of electron structure of atoms and mobility of conduction electron. The electron coherence length in metals increases as the strain increases for all the metals whose electron coherence length is computed and studied due to the deviation in the electron propagation factor from their equilibrium position when strain is applied. Zulkharnay and May (2023) presented a report on the in situ observation of large Negative electron affinity (NEA) from scandium-terminated diamond by depositing monolayer of Scandium (Sc) via electron beam evaporation onto bare diamond (100) and (111) surfaces. The variations of surface structure, electron affinity (EA) and work function (WF) were measured following each annealing step in vacuo at different temperature. Result obtained show that these two Scandium–diamond surfaces have the highest negative electron affinity for metal adsorbed onto bare diamond measured to date. This study also unveils structural and electronic insights into tuning the adsorbate–diamond interface and further expands the potential candidate material map for effective electron-emission applications. Adesakin (2017) used a generalized model developed by Kumar and Singh (2010) for computing the refractive index and energy band gap of different semiconducting material to investigate the effect of linear deformation on refractive index of metals based on free electron theory. The electron density parameters of deformed metals under the application of different strains were obtained for different metals. The result obtained revealed that the refractive index of metals increases as the electron density parameter increases with metals in high density region having low refractive index while

metals in low density region has high refractive index due to the fact that refractive index of metals depend on electronic concentration. There is a good agreement between experimental and computed value of refractive index. The refractive index of all the metals investigated increases as deformation increases. This increase in refractive index could be due to an increase in interatomic spacing between the electrons in metals which forces the refractive index of the metals to increase as deformation increases. Espíndola et.al. (2020) systematically computed the negative electron affinities from ground-state density functional methods using lowest unoccupied molecular orbital energy shift and second-order perturbation calculation of the derivative discontinuity. The results obtained show the importance of asymptotic behavior of exchange-correlation potential in the calculation of negative electron affinities as well as demonstrating the versatility of the nearly correct asymptotic potential NCAP functional. Seidl et. al.,(1998) theoretically computed asymptotic ionization energy and electron affinity of metals based on quantum size correction using restricted-variational electronic density profiles. The result obtained agree quite well with experimental value. They also discuss how many excess electrons can be bound by a neutral cluster of given size in a continuum picture, the criterion for total-energy stability of a negatively charged cluster is less stringent than that for existence of a self-consistent solution. Gutsev and Bauschlicher (2003) computed the electronic and geometrical structures of homo-nuclear metal as well as their anions and cations using density functional theory with six generalized gradient approximations for exchange-correlation potential. The result obtained for adiabatic electron affinities and ionization energies are in good agreement with experimental value when compared. In this work, electron approximation theory is extended to the study of electron affinity of metal. The metals were chosen based on physical constants required for computation and technological applications.

### Theoretical Considerations

Consider a system of ions with the position vector  $\vec{R}_p$ , masses  $M_p$ , charges  $Z_p e$  and valence electron  $r_j$ ,  $m_e$  and –e described by Hamiltonian operator.

$$\hat{H} = -\frac{\hbar^2}{2m_e} \sum_j \nabla_j^2 - \sum_p \frac{\hbar^2}{2M_p} \nabla_p^2 + \frac{1}{2} \sum_j \sum_{k \neq j} \frac{e_j^2}{r_{jk}} - \sum_j \sum_p \frac{Z_p e_j^2}{|r_j - R_p|} + \frac{1}{2} \sum_p \sum_{q \neq p} \frac{Z_p Z_q e_0^2}{R_{pq}} = -\frac{\hbar^2}{2m_e} \sum_j \nabla_j^2 - \sum_p \frac{\hbar^2}{2M_p} \nabla_p^2 + u_{ee}(\vec{r}) + u_{ei}(\vec{r}, \vec{R}) + u_{ii}(\vec{R}) \quad (1)$$

The first two terms describe the kinetic energy, where p is a running index over all the ions, the index j extends over all the electrons whereas  $u_{ee}(\vec{r})$ ,  $u_{ei}(\vec{r}, \vec{R})$  and  $u_{ii}(\vec{R})$  are the potential energies of the electron-electron, electron-ion

and ion-ion interaction respectively, expressed in terms of  $e_o = e/\sqrt{4\pi\epsilon_o}$ . In the Schrodinger equation for the system of atoms, the motion of the valence electrons may be separated from that of the ions by introducing equation (1) the Hamiltonian  $\hat{H}_e$  which describes the electron motion for a set of fixed ionic positions denoted collectively by  $\vec{R}$  in the form

$$\hat{H} \Phi(\vec{r}, \vec{R}) = \left[ \hat{H}_e - \sum_p \frac{\hbar^2}{2M_p} \nabla_p^2 \right] \Phi(\vec{r}, \vec{R}) = E \Phi(\vec{r}, \vec{R}) \quad (2)$$

The eigen value problem for the electronic motion is

$$\hat{H}_e \varphi(\vec{r}, \vec{R}) = \left[ -\frac{\hbar^2}{2m_e} \sum_j \nabla_j^2 + u_{ee}(\vec{r}) + u_{ei}(\vec{r}, \vec{R}) + u_{ii}(\vec{R}) \right] \varphi(\vec{r}, \vec{R}) = E(\vec{R}) \varphi(\vec{r}, \vec{R}) \quad (3)$$

Where  $\psi(\vec{r}, \vec{R})$  and  $E(\vec{R})$  are the eigenfunctions and eigenvalues of  $\hat{H}_e$  with  $\vec{R}$  as a fixed parameter. The electron coordinates denoted collectively by  $\vec{r}$  are the dynamical variables in equation (3). Assuming that the eigenfunctions  $\psi(\vec{r}, \vec{R})$  is known, the wave functions  $\Phi(\vec{r}, \vec{R})$  which solve the Schrodinger equation (2) is approximated by the expression

$$\Phi(\vec{r}, \vec{R}) = \psi(\vec{r}, \vec{R}) \varphi(\vec{R}) \quad (4)$$

Known as adiabatic approximation. Substituting equation (4) into equation (2) we have

$$-\sum_p \frac{\hbar^2}{2M_p} [\varphi(\vec{R}) \nabla_p^2 \psi(\vec{r}, \vec{R}) + 2\nabla_p \psi(\vec{r}, \vec{R}) \cdot \nabla_p \varphi(\vec{R}) + \psi(\vec{r}, \vec{R}) \nabla_p^2 \varphi(\vec{R})] + E(\vec{R}) \psi(\vec{r}, \vec{R}) \varphi(\vec{R}) = E \psi(\vec{r}, \vec{R}) \varphi(\vec{R}) \quad (5)$$

By multiplying the left of each term in equation (5) by  $\psi^*(\vec{r}, \vec{R})$  and integrating over all electron positions, we obtain an equation for  $\varphi(\vec{R})$

$$-\sum_p \frac{\hbar^2}{2M_p} \nabla_p^2 \varphi(\vec{R}) + E(\vec{R}) \varphi(\vec{R}) = E \varphi(\vec{R}) + \sum_p \frac{\hbar^2}{2M_p} S \varphi(\vec{R}) \int \psi^*(\vec{r}, \vec{R}) \nabla_p^2 \psi(\vec{r}, \vec{R}) d\vec{r} + \sum_p \frac{\hbar^2}{M_p} \nabla_p \varphi(\vec{R}) \int \psi^*(\vec{r}, \vec{R}) \nabla_p \psi(\vec{r}, \vec{R}) d\vec{r} \quad (6)$$

Where the electron Eigen functions are assumed to be normalized. If the valence electrons can be considered perfectly free, the last two terms on the right-hand side vanish because  $\psi(\vec{r}, \vec{R})$  becomes independent of the ion coordinates  $\vec{R}$  so that  $\nabla_p \psi(\vec{r}, \vec{R})$  is zero.

If electron number per mole is  $N_0$ , the Fermi radius  $K_F$  is obtained as

$$K_F = \left[ 3\pi^2 \left( \frac{N_0}{V} \right) \right]^{1/3} \quad (7)$$

where  $V$  is volume. The Fermi energy  $E_F$  of free electron with Fermi radius  $K_F$  is

$$E_F = \frac{\hbar^2 K_F^2}{2m} = \left( \frac{\hbar^2}{2m} \right) \left[ 3\pi^2 \left( \frac{N}{V} \right) \right]^{2/3} \quad (8)$$

Due to presence of potential  $U(r)$ , equation (8) is modified as

$$E_F + U(r) = \left( \frac{\hbar^2}{2m} \right) [3\pi^2 \rho(r)]^{2/3} \quad (9)$$

And

$$\rho(r) = \left(\frac{1}{3\pi^2}\right) \left(\frac{2m}{\hbar^2}\right)^{3/2} E_F^{3/2} \left[1 + \frac{U(r)}{E_F}\right]^{3/2} \quad (10)$$

The electron affinity of metals is obtained as

$$\frac{9e_0^2}{10} \left[ \frac{2.45a_0}{2r_s^2} - \frac{1}{r_s} \right] - \frac{50.1}{r_s^2} \quad (11)$$

Where  $a_0$  is Bohr radius,  $e_0 = e/\sqrt{4\pi\epsilon_0}$ ,  $e$  is electronic charge,  $\epsilon_0$  is permittivity of free space and  $r_s$  is the electron density parameter.

In this work, electron affinity of metals is computed and studied using equation (11). Metals were chosen from various groups and periods.

### Results and Discussion

Figure 1 shows the plot of electron affinity against electron density parameter for alkali, earth alkaline, group three, noble and transition metals. Result obtained in figure 1 revealed that electron affinity of metals increases as the electron density parameter increases. This increase may be due to change in atomic radius, nuclear charge and electronic configuration of metals. The pattern display by metals in figure 1 seems to suggest that electron affinity of metals depend on the ratio of the number of valence electron per unit volume as metals in the region of high density limit have low electron affinity than metals in the region of high density limit. There is a good agreement between the computed and ab-initio value of electron affinity of metals in figure 1 because the more negative the electron affinity value, the higher an atom's affinity for electrons. The ab-initio value is obtained by directly substituting the experimental value of Fermi energy obtained from solid state Physics by Ashcroft and Mermin (1976) into the model used for computation. The trend display by metals in figure 1 also revealed that electron affinity of metals relied on density of valence electron and electronic concentration of metals since most of the metals whose electron affinity were computed and studied concentrated more in the region of high density limit than low density limit. The result obtained for electron affinity in this work is negative. This may be due to the fact that electron affinity is the energy released when electron binds to an atom and also the quantitative measurement of the energy change that results from adding a new electron to a neutral atom. Furthermore, the low value of electron affinity poses by metals in the region of high density limit could be due to its high conductivity (metals) nature of metals while high value of electron affinity poses by metals in the region of low density limit could be due to its low conductivity (non-metals) nature of metals. Figure 2 shows the plot of electron affinity against electron density parameter for metals belonging to different elemental group and period. In figure 2, electron affinity of metals rises as strain increases. This increase is caused by change in band structure and energy levels of electrons in metals. In figure 2, increase in electron affinity of metals as strain increases can be caused by heavy distortion in lattice parameters in the core shell of the metals and splitting of electron valence band. Furthermore, the increase in the electron affinity of metals as strain increases in figure 2 could be due to the fact that the contact energy barrier between the electrons in the metals is lowered as the strain increases.

### Conclusion

In summary, we have used electron approximation theory to theoretically study electron affinity of metals. The result obtained for electron affinity in this work is negative. This may be due to the fact that electron affinity is the quantitative measurement of the energy change that results from adding a new electron to a neutral atom. There is a good agreement between the computed and ab-initio value of electron affinity. The electron affinity of metals increases as the electron density parameter increases. The increase in electron affinity of metals as strain increases can be caused by heavy distortion in lattice parameters in the core shell of the metals and splitting of electron valence band.

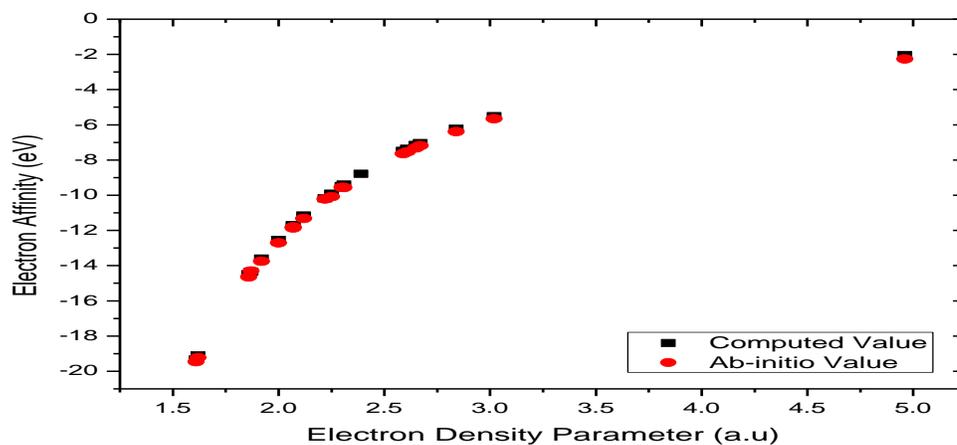
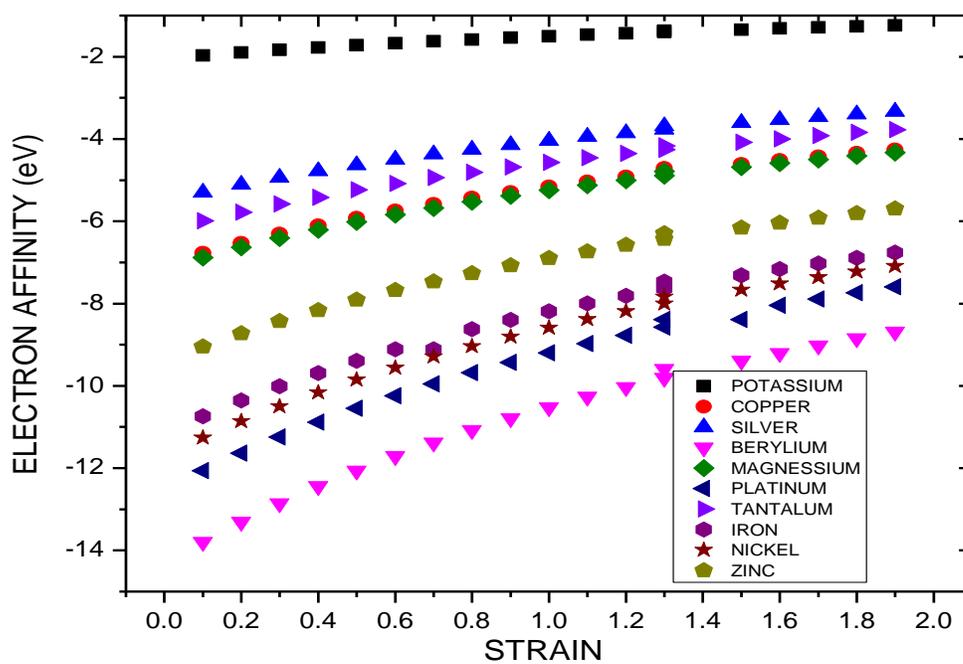


FIGURE 1: Electron Affinity Plotted Against Electron Density Parameter of Metals



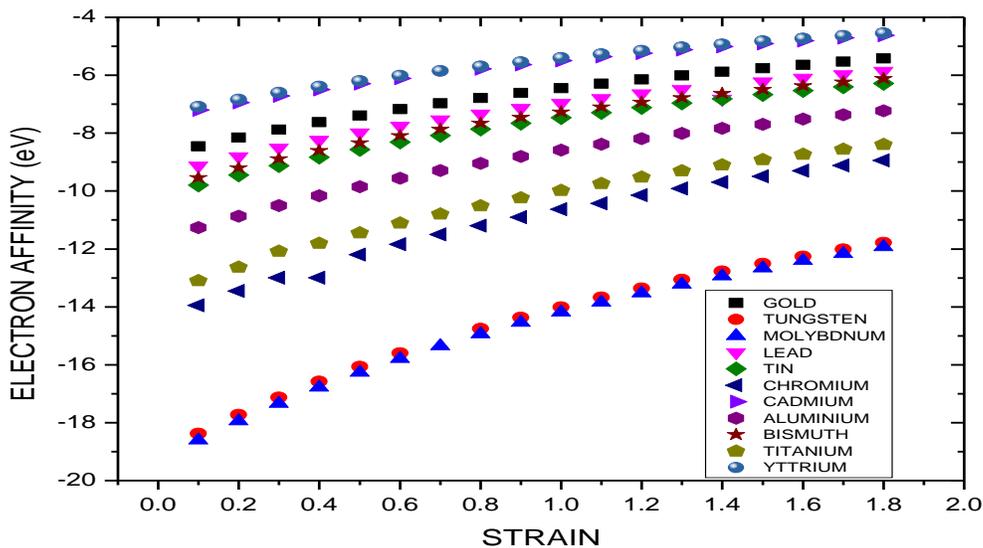


Figure 2: Electron Affinity Plotted against Strain for Metals

Table 1: Electron Affinity of Metals

Metals	Electron Density Parameter $r_s$ (a.u)	Computed Electron Affinity (eV)	Ab-initio Electron Affinity (eV)
K	4.96	-2.04732	-2.25848
Cu	2.67	-7.04225	-7.18237
Ag	3.02	-5.50727	-5.65706
Be	1.87	-14.3402	-14.3070
Mg	2.65	-7.14874	-7.31262
Cr	1.86	-14.4946	-14.6452
Fe	2.12	-11.1615	-11.3292
Ni	2.07	-11.7063	-11.8675
Zn	2.31	-9.40344	-9.57300
Cd	2.59	-7.48315	-7.64313
Al	2.07	-11.7063	-11.8077
Bi	2.25	-9.91079	-10.0822
Ti	1.92	-13.6040	-13.7597
Y	2.61	-7.36912	-7.53298
Sn	2.22	-10.1800	-10.2120

Pb	2.30	-9.48525	-9.55302
Mo	1.61	-19.3386	-19.4637
W	1.62	-19.1009	-19.2255
Au	2.39	-8.78546	-5.68722
Pt	2.00	-12.5389	-12.7044
Ta	2.84	-6.22590	-6.39020

.. Table 2: Electron Affinity of Strained Metals

Metal	Electron Density Parameter	Strain								
		0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8
K	4.96	-1.9003	-1.7773	-1.6726	-1.5821	-1.5031	-1.4333	-1.3712	-1.3154	-1.2650
Cu	2.67	-6.5357	-6.1119	-5.7511	-5.4396	-5.1674	-4.9270	-4.7130	-4.5210	-4.3475
Ag	3.02	-5.1112	-4.7799	-4.4978	-4.2542	-4.0414	-3.8535	-3.6862	-3.5360	-3.4004
Be	1.87	-13.308	-12.445	-11.710	-11.075	-10.520	-10.031	-9.5947	-9.2035	-8.8501
Mg	2.65	-6.6345	-6.2043	-5.8381	-5.5218	-5.2455	-5.0015	-4.7843	-4.5893	-4.4132
Cr	1.86	-13.451	-12.997	-11.836	-11.194	-10.634	-10.139	-9.6980	-9.3026	-8.9454
Fe	2.12	-10.358	-9.686	-9.1143	-8.6205	-8.1888	-7.8081	-7.4685	-7.1641	-6.8890
Ni	2.07	-10.863	-10.160	-9.5592	-9.0412	-8.5885	-8.1889	-7.833	-7.5136	-7.2252
Zn	2.31	-8.7268	-8.1608	-7.6790	-7.2629	-6.8994	-6.5784	-6.2948	-6.0361	-5.8044
Cd	2.59	-6.9448	-6.4945	-6.1111	-5.7801	-5.4908	-5.2354	-5.0080	-4.8039	-4.6196
Al	2.07	-10.864	-10.159	-9.5592	-9.0412	-8.5885	-8.1889	-7.8330	-7.5136	-7.2252
Bi	2.25	-9.1977	-8.6011	-8.0932	-7.6547	-7.2715	-6.9332	-6.6319	-6.3616	-6.1174
Ti	1.92	-12.625	-11.806	-11.109	-10.507	-9.9804	-9.5160	-9.1023	-8.7312	-8.3959
Y	2.61	-6.8390	-6.3955	-6.0180	-5.6920	-5.4071	-5.1557	-4.9317	-4.7308	-4.5492
Sn	2.22	-9.4474	-8.8347	-8.3130	-7.8626	-7.4690	-7.1215	-6.8120	-6.5343	-6.2835
Pb	2.30	-8.8027	-8.2318	-7.7458	-7.3261	-6.9593	-6.6356	-6.8120	-6.0886	-5.8549
Mo	1.61	-17.947	-16.782	-15.791	-14.934	-14.186	-13.526	-12.938	-12.410	-11.934
W	1.62	-17.726	-16.576	-15.596	-14.750	-14.012	-13.360	-12.779	-12.258	-11.787
Au	2.39	-8.1534	-7.6245	-7.1744	-6.7857	-6.4460	-6.1462	-5.8792	-5.6395	-5.4230
Pt	2.00	-11.637	-10.882	-10.239	-9.6841	-9.1992	-8.7710	-8.3899	-8.0478	-7.7388
Ta	2.84	-5.7781	-5.4212	-5.0846	-4.8092	-4.5686	-4.3561	-4.1669	-3.9971	-3.8438

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