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Birds of a Feather Flock Together (On the Similarity of Gold and Phosphorus Alignment Energies)

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Abstract: *Blue phosphorene configuration of P_9, P_{16} and P_{25} clusters on an Au (111) surface coincides with the similarity of gold and phosphorus alignment energies.*

Keywords: *P_9, P_{16} and P_{25} clusters on an Au (111) surface, gold and phosphorus alignment energies*

1. INTRODUCTION

Tian et al [1] fabricated two-dimensional metal-phosphorus networks on an Au (111) substrate, namely, on gold with an atomically flat close-packed face-centred-cubic (fcc) surface. The networks were composed of phosphorus subunits such as P_9, P_{16}, and P_{25}, which were glued together by gold atoms. (See Figure 1) [1].

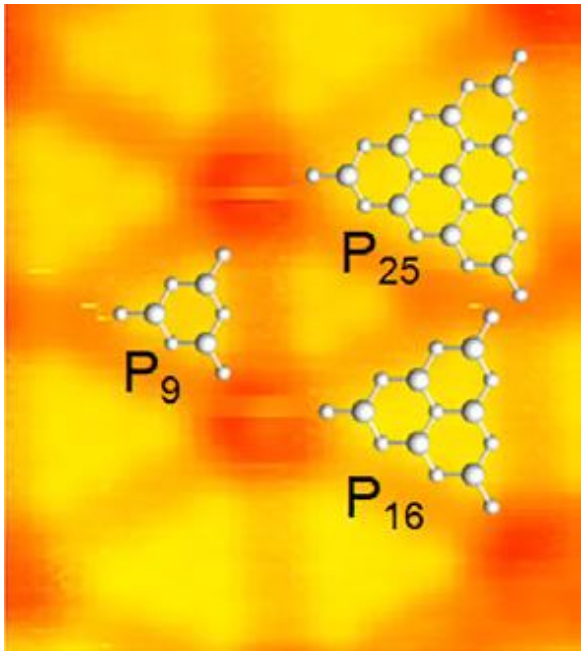

Figure1. *Phosphorus subunits P_9, P_{16} and P_{25} glued together by gold atoms*

Strikingly [2], these subunits were synthesized ‘‘on spot,’’ namely, during the fabrication process, rather than being pre-selected. Even the gold atom linkers were supplied on spot, namely, handily extracted from the more weakly bonded steps of the vicinal Au (111) substrate.

A pictorial representation of the atomistic growth mechanism is illustrated in Figure 2 [2]. Individual P atoms are deposited onto the stepped Au (111) surface and migrate to form islands (Figure 2A).

As the islands grow in size, they may adopt the energetically more favourable blue phosphorene configuration. In particular, the islands of P_9, P_{16}, and P_{25} containing respectively one, three, and six complete hexagons should be highly preferred and more abundantly prepared at the surface (see Figure 2B). To further sew these islands, known as magic clusters, into a complete network on Au (111) at higher phosphorus coverages, extra help is needed, as provided by the linking Au atoms extracted from the steps (shown in Figure 2C and 2D for the case of the P_9 islands).

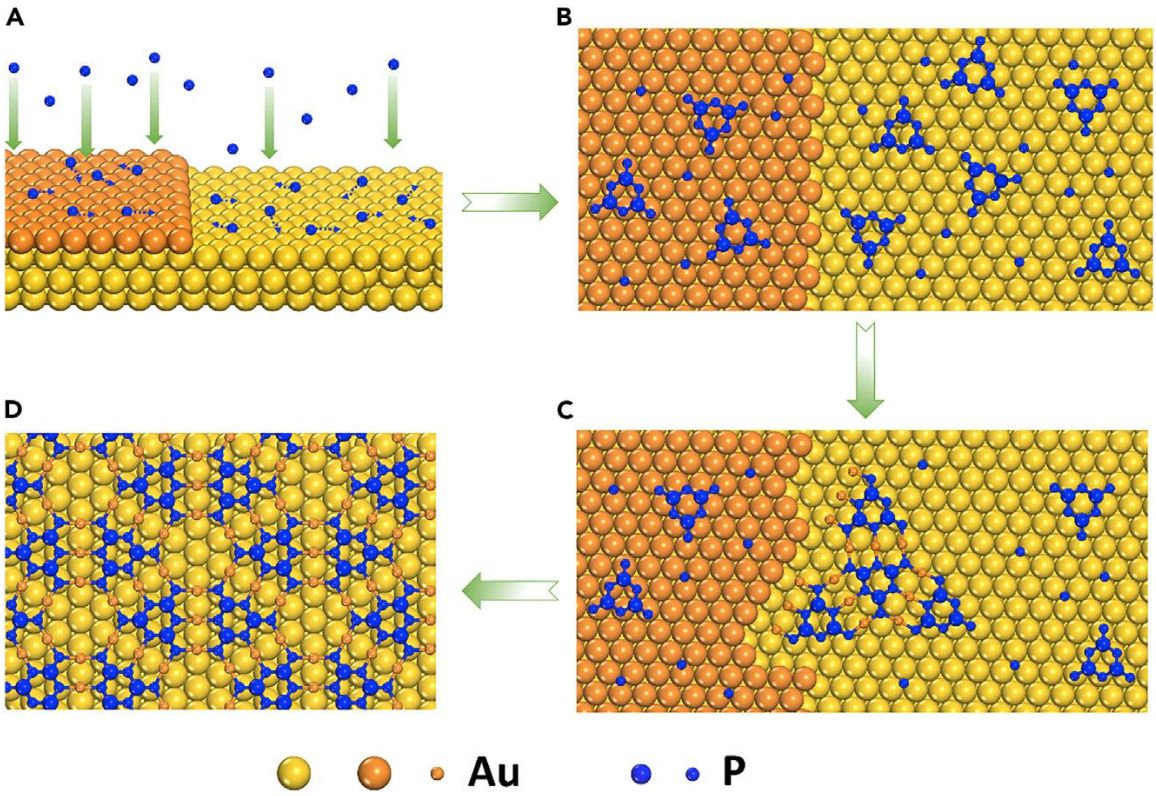

Figure2. *A Pictorial Representation of the Atomistic Growth Mechanism of Two-Dimensional Metal-Phosphorus Networks on Au (111):*

(A) Deposition and diffusion of phosphorus atoms.

(B) On-spot formation of magic P_9 clusters.

(C) Linking of the P_9 clusters by the Au atoms extracted from the steps.

(D) Completion of a two-dimensional metal-phosphorus network.

Let us see how the energetically more favourable blue phosphorene configuration of P_9, P_{16} and P_{25} clusters on an Au (111) surface coincides with the similarity of gold and phosphorus alignment energies.

2. THE ALIGNMENT ENERGY

The alignment energy of the atom or molecule and even cluster enables the alignment of the electron with its atom or molecule or cluster nature [3], [4],[5],[6],[7],[8],[9],[10],[11]. The next formula should be applicable also for gold and phosphorus atoms and their clusters:

$$Wk_{alignment} = \left(\frac{R_{unaligned}}{R_{aligned}} - 1\right) m_{electron}^{rest} c^2. \quad (1)$$

Where $R_{unaligned}$ in our present case is the unaligned modified ratio of gold or phosphorus atom or cluster mass to electron mass:

$$R_{unaligned} = \frac{m_{atom\ or\ cluster}}{m_{electron}^{rest}}\ s(1). \quad (2)$$

The rest mass of the electron can be expressed in daltons (Da), i.e. $m_{electron}^{rest} =$ 0,00054857990907 Da. The factor *s(1) = 1,696 685 529…* is the average elliptic-hyperbolic manifestation of one (n = 1) elliptic Compton wavelength of the electron given by the next equation:

$$s(n) = n\left(2 - \frac{1}{\sqrt{1+\frac{\pi^2}{n^2}}}\right), n \in \mathbb{N}. \quad (3)$$

And the aligned modified ratio $R_{aligned}$ is given by the same equation (3) for the down rounded unaligned modified ratio (n=*ROUNDDOWN* ($R_{unaligned}$)) as follows:

$$R_{aligned} = s\left(\text{ROUNDDOWN}\left(R_{unaligned}\right)\right). \quad (4)$$

3. The Gold and Phosphorus Alignment Energies

Using the data from the reference [12], [13] and applying the equations (1), (2), (3), (4) the alignment energies of gold atom Au and first four gold clusters Au_2, Au_3, Au_4 and Au_5 as well the alignment energies of phosphorus clusters P_9, P_{16} and P_{25} have been calculated and presented in Table 1.

Table1. *Some similar alignment energies of gold (Au, Au_2, Au_5) and phosphorus (P_9, P_{16}, P_{25}), respectively*

Gold	Mass (Da)	R unaligned	R aligned	Alignment energy (eV)
Au	**196,966570**	**609191,703250**	**609191,000008**	**0,589890075**
Au_2	**393,933140**	**1218383,406499**	**1218383,000004**	**0,170487202**
Au_3	590,899710	1827575,109749	1827575,000003	0,030685643
Au_4	787,866280	2436766,812999	2436766,000002	0,170488476
Au_5	**984,832851**	**3045958,516249**	**3045958,000002**	**0,086607118**
Phosphorus	Mass (Da)	R unaligned	R aligned	Alignment energy (eV)
P_9	278,763867	862179,987477	862179,000006	0,585257570
P_{16}	495,580208	1532764,422181	1532764,000003	0,140747418
P_{25}	774,344075	2394944,409658	2394944,000002	0,087406607

From the Table 1 we can see the next similar alignment energies of gold and phosphorus coinciding with the formation of phosphorus clusters on the gold surface:

a) Alignment energy of gold Au approximately equals the alignment energy of phosphorus cluster P_9:

$$W_{alignment}^{Au} = 0{,}589890075eV \approx 0{,}585257570eV = W_{alignment}^{P9}. \quad (5a)$$

b) Alignment energy of gold cluster Au_2 almost equals the alignment energy of phosphorus cluster P_{16}:

$$W_{alignment}^{Au2} = 0{,}170487202eV \approx 0{,}140747418 = W_{alignment}^{P16}. \quad (5b)$$

c) Alignment energy of gold cluster Au_5 approximately equals the alignment energy of phosphorus cluster P_{25}:

$$W_{alignment}^{Au5} = 0{,}086607118eV \approx 0{,}087406607eV = W_{alignment}^{P25}. \quad (5c)$$

d) Alignment energy of gold cluster Au_2 approximately equals the sum of the alignment energy of phosphorus cluster P_{16} and the alignment energy of gold cluster Au_3:

$$W_{alignment}^{Au2} = 0{,}170487202eV \approx 0{,}171433061eV = W_{alignment}^{P16} + W_{alignment}^{Au3}. \quad (5d)$$

4. Conclusion

It seems that even in the micro world, the next proverb is followed: "Birds of a feather flock together"

Dedication

To the Slovene version of the proverb which reads: “Gliha vkup štriha”

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