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Subtle Anti-bonding Orbits of Methane (Yin Yang Trick)

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Abstract: *Yin yang characteristics of methane arepresented.*

Keywords: *subtle bond,methane molecule,carbon andhydrogen atom, adsorption energy*

1. Introduction

In the previous article, a stable subtle bond between unequal atoms of the same molecule was presented on the example of some hydrides of the sixth group of elements.[1]In this paper, we will continue the exercise on the example of methane molecule, where a geometrically stable subtle bond between atoms is not present.The necessary data are again taken from reference [2]

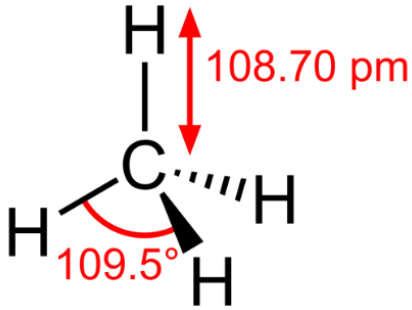

Figure1. *The methane molecule*

Toput them in the key formulathat relates the length on the elliptic surface $n$and the length on the average elliptic-hyperbolic surface $s(n)$as follows [1]:

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

2. No Subtle Bonding betweenCarbon Atom Cand Hydrogen Atom H in Methane Molecule CH_4

The distance$d_{CH\ in\ CH4}^{measured}$ measured between the carbon atom $C$and the hydrogen atom H in the methane molecule$CH_4$is $108.70\,pm$ [2].This expressed in Compton wavelengths of the electron equals $d_{CH\ in\ CH4}^{measured} = 44.801\,\lambda_e$. The πtimes longer orbit length of $s_{CH\ in\ CH4}^{measured} = 140.745\,\lambda_e$ is near to the geometrically unstable orbit length of $s(140.5\,\lambda_e) = 140.504\,\lambda_e$.(1)And the doubled value $2s_{CH\ in\ CH4}^{measured} = 281.490\,\lambda_e$ is close to the geometrically unstable orbit lengthof$s(281.5\,\lambda_e) = 281.518\,\lambda_e$.(1) So, it shows that the stable subtle CH bonding orbit between carbon atom C and hydrogen atoms H in methane molecule CH_4 is not formed.Anyway, if it occurs, it is very short-lived.

3. Subtle Anti-Bonding Orbits between Carbon Atom C and Hydrogen Atom H in Methane Molecule CH_4

As noted in the previous section 2 the subtle bonding between carbon atom C and hydrogen atom H in methane molecule $CH_4$is short-lived because the measured value of the doubled orbit of $2s_{CH\ in\ CH4}^{measured} = 281.490\,\lambda_e$ is close to thegeometricallyunstable doubled orbit length of $s(281.5\,\lambda_e) = 281.518\,\lambda_e(1)$.On the contrary, the yin yang combination of the antibonding orbit of carbon atom C and the anti-bonding orbit of hydrogen atom Hcan bypass the geometric instability.For thispurpose, thedoubled elliptic length of$2n_{CH} = 281.5\,\lambda_e$is divided to the doubled carbon orbit length$2n_C$on one side,and to the doubled hydrogen orbit length$2n_H$on the other side, by consideringthat theassigned

length is inversely proportional to the electronegativityof the carbon atom $e_C = 2.55$ and electronegativity of the hydrogen atom$e_H = 2.2$. [3]

Yielding the doubled elliptic orbitlength$2n_C$ofthe carbon C as follows:

$$2n_C = \frac{2.2}{2.55 + 2.2}.281.5\ \lambda_e = 130{,}378\ 947\ \lambda_e. \quad (2)$$

And

Yielding the doubled elliptic orbit length $2n_H$of the hydrogen H as follows:

$$2n_H = \frac{2.55}{2.55 + 2.2}.281.5\ \lambda_e = 151{,}121\ 053\ \lambda_e. \quad (3)$$

Both unstable individual doubled orbits $2n_C$and $2n_H$become geometrically stable with a trickwhere the electron wave retreats to an adjacent orbit before annihilating in the native orbit.

4. Energy Cost of Forming Anti-bonding Orbits from Bonding Orbit between Carbon Atom C and Hydrogen Atom H in Methane Molecule CH_4

For calculating energy cost of forming anti-bonding orbits the original orbitsn_C and $n_H$and n_{CH}instead of doubled ones$2n_C$ and $2n_H$and$2n_{CH}$should be taken into account.

The original orbit length$n_C$belonging to the carbon atom C:

$$n_C = \frac{2n_C}{2} = \frac{130{,}378\ 947\ \lambda_e}{2} = 65{,}189\ 474\ \lambda_e\ \ and\ \ s(n_c) = 65{,}265\ 041\ \lambda_e\ . \quad (4)$$

The original orbit length$n_H$belonging to the hydrogen atom H:

$$n_H = \frac{2n_H}{2} = \frac{151{,}121\ 053}{2} = 75{,}560\ 527\ \lambda_e\ \ and\ \ s(n_H) = 75{,}625\ 752\ \lambda_e. \quad (5)$$

The sum $n_{CH}$of the original orbit length of the carbon atom C and the original orbit length of the hydrogen atom H:

$$n_{CH} = \frac{2n_{CH}}{2} = \frac{281.50\ \lambda_e}{2} = 140.75\ \lambda_e\ \ and\ \ s(n_{CH}) = 140{,}785\ 048\ \lambda_e. \quad (6)$$

Then taking into account that the curved bonding distance is half of the orbit lengthit holds for the energy of forming anti-bonding orbits from the bonding orbit[4]:

$$\Delta E_{forming}^{anti-bonding} = 2Ry.\alpha^{-1}\left(-\frac{1}{s(n_c) + s(n_H)} + \frac{1}{s(n_{CH})}\right). \quad (7)$$

Applying$Ry = 13.605\ 693\ 009\ eV$ and $\alpha^{-1} = 137.035\ 999\ 146$and inserting data we get:

$$\Delta E_{forming}^{anti-bonding} = 0{,}019\ 88\ eV = +0.02\ eV. \quad (8)$$

This energy should be invested (signed positive) for forming subtle anti-bonding orbits from the bonding orbit between the carbon atom C and the hydrogen atom H in the methane molecule CH_4. And it could be released (signed negative) at an exothermic adsorption of methane moleculeCH_4 to some surface.

5. Mining Result

The HCP (Hexagonal Close Packed) hollow site ofNi2Cu overlayer of Ni (111) is such a surface. Since CH_4 species was physically adsorbed at it with a weak adsorption energy of −0.02 eV. [5]

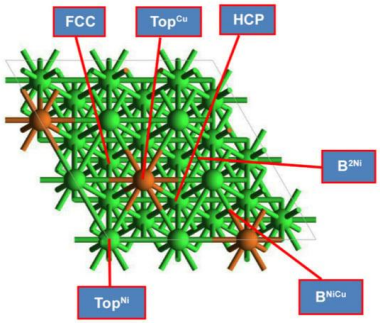

Figure 2.Schematic illustration of Ni_2Cu overlayer of Ni (111) surface. FCC, HCP, Top^{Ni}, Top^{Cu}, B^{2Ni}, and B^{NiCu} represent a face centered cubic, hexagonal close packed, Ni at the top site, Cu at the top site,

Ni–Ni at the bridge site and Ni–Cu at the bridge site, respectively. Green and brown spheres represent Ni and Cu atoms, respectively. [5]

6. CONCLUSION

Surface is O.K. But one still doesn't know for sure what is hidden behind it.

DEDICATION

To Plato and his quote

Figure3. *Opinion*

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ADDENDUM

Let’s check the subtle bond between hydrogen atoms H in methane molecule CH_4, too.

A. No Subtle Bonding between Hydrogen Atoms H in Methane Molecule CH_4

The distance $d_{HH\ in\ CH4}^{measured}$ measured between the hydrogen atoms H in the methane molecule CH_4yields177.51 $pm = 73.160\ \lambda_e$. The π times longer orbit length of $s_{HH\ in\ CH4}^{measured} = 229.840\ \lambda_e$ is near to the geometrically unstable orbit length of $s(229.5\ \lambda_e) = 229.521\ \lambda_e$. (1)And the doubled value $2s_{HH\ in\ CH4}^{measured} = 459.681\ \lambda_e$ is close to the geometrically unstable orbit length of $s(459.5\ \lambda_e) = 459.511\ \lambda_e$. (1) So, it shows that the stable subtle HH bonding orbit between hydrogen atoms H in methane molecule CH_4 is not formed. Anyway, if it occurs, it is very short-lived.

B. Subtle Anti-Bonding Orbits between Hydrogen Atoms H in Methane Molecule CH_4

On the contrary, the yin yang combination of the antibonding orbit of hydrogen atoms H can bypass the geometric instability. For this purpose, the doubled elliptic length of $2n_{HH} = 459.5\ \lambda_e$ is equally divided to both adjacent hydrogen atoms yielding

$$n_{HH} = 2n_H = \frac{2n_{HH}}{2} = \frac{459.5\ \lambda_e}{2} = 229.75\ \lambda_e \quad and\ s(n_{HH}) = 229{,}771\ 476\ \lambda_e. \qquad (a)$$

And

$$n_H = \frac{n_{HH}}{2} = \frac{229.75\ \lambda_e}{2} = 114{,}875\ \lambda_e \quad and\ s(n_H) = 114{,}917\ 934\ \lambda_e. \qquad (b)$$

Both unstable individual doubled hydrogen orbits $2n_H$ become geometrically stable with a trick where the electron wave retreats to an adjacent hydrogen orbit before annihilating in the native hydrogen orbit.

For calculating energy cost of forming anti-bonding orbits the original orbits $n_H = 114.875\ \lambda_e$ and $n_{HH} = 2n_H = 229.75\ \lambda_e$ should be taken into account. And also the fact that the curved bonding distance is half of the orbit length. The next relation is given:

$$\Delta E_{forming}^{anti-bonding} = 2Ry.\alpha^{-1}\left(-\frac{1}{s(n_H)+s(n_H)} + \frac{1}{s(n_{HH})}\right). \qquad (c)$$

That can be written in a simplified form:

$$\Delta E_{forming}^{anti-bonding} = Ry.\alpha^{-1}\left(-\frac{1}{s\left(\frac{n_{HH}}{2}\right)} + \frac{1}{\frac{s(n_{HH})}{2}}\right). \qquad (d)$$

Where in our case $n_{HH} = 229.75\ \lambda_e$ is available. Then applying $Ry = 13.605\ 693\ 009\ eV$ as well as $\alpha^{-1} = 137.035\ 999\ 146$ and inserting needed data the next result is given:

$$\Delta E_{forming}^{anti-bonding} = 0{,}004\ 547\ eV = +0.0045\ eV. \qquad (e)$$

C. Mining Result

Its frequency equivalent 1099 GHz is near to the value of the known methane line at 1256 GHz.[6]

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