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Decrease of Preserved Kinetic Energy of Electron at Ultra-high Hydrogen Storage (Case Report)

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Abstract: *The preserved kinetic energy of the electron decreases during the transition from the Hydrogen molecule orbit to the Hydrogen atom orbit..*

Keywords: *Preserved kinetic energy of the electron, Hydrogen adsorption on Li-decorated holey graphyne (HGY)*

1. INTRODUCTION

In previous paper [1] was proposed that the non-preserved kinetic energy of the electron is converted to orbital distribution energy and so expresses the orbital affiliation; on the other hand the preserved kinetic energy of the electron plays a role of the electron character in any atom or molecule orbit. In a way that the part of this energy should be always the same:

$$\Delta_{preserved} = \frac{W_{preserved}}{W_{original\ kinetic}} = 0.1198. \qquad (1)$$

But its absolute value should depend on the amount of the original kinetic energy of the electron:

$$W_{preserved} = \Delta_{preserved} W_{original\ kinetic}. \qquad (2)$$

The original kinetic energy of the electron equals the ionization energy, so we can write:

$$W_{preserved} = \Delta_{preserved} W_{ionization}. \qquad (3)$$

Let's find an example. The closest is the Hydrogen atom to look at, and the next is the Hydrogen molecule.

2. THE PRESERVED KINETIC ENERGY OF THE ELECTRON IN THE HYDROGEN ATOM H AND THE MOLECULE H2

The measured ionization energy of Hydrogen atom H and Hydrogen molecule H_2 is 13.60 and 15.42eV, respectively. [2] So, applying the relation (3) the corresponding preserved kinetic energy of the electron is found. For the Hydrogen atom H it holds:

$$W^{H}_{preserved} = 0.1198\ x\ 13.60\ \text{eV} = 1.63\ eV. \qquad (4)$$

And for the Hydrogen molecule H_2 we have:

$$W^{H_2}_{preserved} = 0.1198\ x\ 15.42\ \text{eV} = 1.85\ eV. \qquad (5)$$

The electron character in the Hydrogen molecule is therefore 0.22 eV richer than that in the Hydrogen atom:

$$\Delta W_{preserved} = W^{H_2}_{preserved} - W^{H}_{preserved} = 0.22\ eV. \qquad (6)$$

This energy should be released during the transition of an electron from a Hydrogen molecule orbit to a Hydrogen atom orbit.

3. THE CASE REPORT

We are witnessing such a release of energy 0.22eV/H2 in the case of the adsorption of Hydrogen molecules on the Li-decorated single-layer of holey graphyne (HGY) which is a promising candidate for ultra-high Hydrogen storage. [3]

4. CONCLUSION

The ultra-high Hydrogen storage capacity of holey graphyne could be achieved with the help of the uniform distribution of electrons in atom and molecule orbit of Hydrogen.

DEDICATION

To the first day of school and discernment [4]

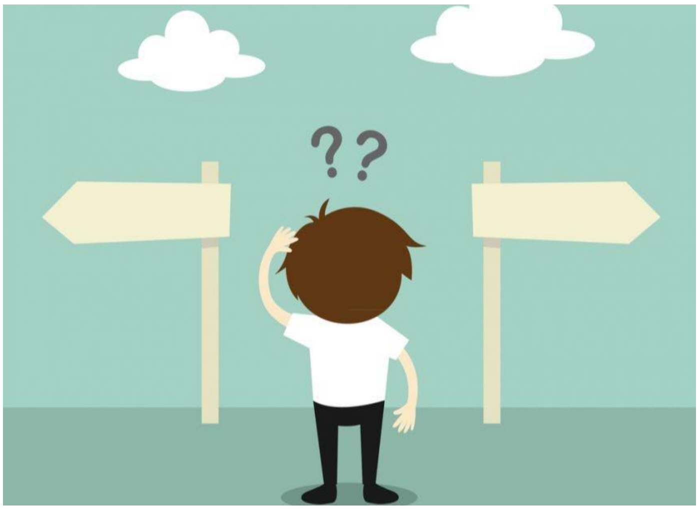

Figure1. *Discernment [4]*

REFERENCES

[1]Janez Špringer (2023) “Adjusted Upper Limit in Mendeleev’s Periodic Table (Flirting of the Micro and Macro world) “International Journal of Advanced Research in Physical Science (IJARPS) 10(8), pp.15- 17, 2023.

[2]https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Atomic_Theory/Ionization_Energies_of_Diatomic_Molecule. Retrieved August 2023

[3]Gao Y, Zhang H, Pan H, Li Q, Zhao J. Ultrahigh hydrogen storage capacity of holey graphyne. Nanotechnology. 2021 Mar 4; 32(21):215402.

[4]https://www.pblcoc.org/thought-for-the-day/discernment-a-key-to-christ-like-living/. Retrieved August 2023

[5]Ray, P. et al. “In situ vibrational spectroscopy of adsorbed nitrogen in porous carbon materials.” *Physical chemistry chemical physics: PCCP* 20 22 (2018): 15411-15418.

[6] https://www.quora.com/Why-is-the-ionisation-energy-of-O-O2. Retrieved Avgust 2023

[7] Fang, Zongtang, Lan Li, David A. Dixon, Rebecca R. Fushimi, and Eric J. Dufek. "Nature of oxygen adsorption on defective carbonaceous materials." The Journal of Physical Chemistry C 125, no. 37 (2021): 20686-20696.

ADDENDUM

In order to test the validity of the theory let's look at another example.

The measured ionization energy of Nitrogen atom N and Nitrogen molecule N_2 is 14.53 and 15.58 eV, respectively. [2] So, applying the relation (3) the corresponding preserved kinetic energy of the electron is found. For the Nitrogen atom N it holds:

$$W_{preserved}^{N} = 0.1198\ x\ 14.53\ \text{eV} = 1.74\ eV. \qquad (a)$$

And for the Nitrogen molecule N_2 we have:

$$W_{preserved}^{N_2} = 0.1198\ x\ 15.58\ \text{eV} = 1.87\ eV. \qquad (b)$$

The electron character in the Nitrogen molecule is therefore 0.13 eV richer than that in the Nitrogen atom:

$$\Delta W_{preserved} = W_{preserved}^{N_2} - W_{preserved}^{N} = 0.13\ eV. \qquad (c)$$

This energy should be released during the transition of an electron from a Nitrogen molecule orbit to a Nitrogen atom orbit. It equals the binding energy of 0.13 eV given by vdW-DFT (van der Waals Density Functional Theory) calculations for a single N_2 molecule adsorbed on graphene as well as is consistent with a compilation of both semi-empirical and experimental data for a single N_2 on graphite, which consistently yield a binding energy of around 0.1 eV.[5]

Homework

One swallow does not bring spring, so let's check further. Oxygen attracts attention, because the measured ionization energy of Oxygen molecule O_2, yielding 1.63 eV, is smaller than the ionization energy of an Oxygen atom O, yielding 13.62 eV. [6] Applying the relation (3) the corresponding preserved kinetic energy of the electron is found. For the Oxygen atom O it holds:

$$W_{preserved}^{O} = 0.1198\ x\ 13.62\ \text{eV} = 1.6317 eV. \qquad (d)$$

And for the Oxygen molecule O_2 we have:

$$W_{preserved}^{O_2} = 0.1198\ x\ 1.63\ \text{eV} = 0.1953\ eV. \qquad (e)$$

The electron character in the Oxygen molecule (e) is therefore regarding common diatomic molecules exceptionally poorer than that in the Oxygen atom (d) as follows:

$$\Delta W_{preserved} = W_{preserved}^{O_2} - W_{preserved}^{O} = -1.44\ eV. \qquad (f)$$

This energy should be invested during the transition of the electron from an Oxygen molecule orbit to an Oxygen atom orbit. What means that adsorption of Oxygen is an endothermic reaction. Indeed, the addition of an Oxygen molecule on graphene leads to the formation of two epoxy groups. This step is endothermic by 1.44 eV. [7]

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