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Study of Chemical Hardness: A Periodic Descriptor

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ABSTRACT

In order to demonstrate a connection between the Physico-compound properties of particles, molecules, and condensed phases of substance, hardness is an important periodic descriptor employed by scientists. Chemical hardness is innately resistant to deformation under perturbation. The electrostatic attraction of the nucleus to the outermost electron of the atom is the conceptual basis for the electronegativity and hardness of a substance. Electronegativity, which has previously been described using the energy and force paradigm. The energy notion has been used by a number of scientists to describe atomic hardness, but the force model for hardness is novel. Given that atomic hardness and atomic electronegativity are found to be in equilibrium, we have defined the hardness as force model for this endeavour. All of the bare minimum requirements for an atomic hardness scale have been met by the new one. The force model's anticipation of the hardness

Keywords: Physico-compound, Chemical hardness, Electronegativity,

INTRODUCTION

Chemical hardness is a fundamental concept in the field of theoretical and computational chemistry that describes the resistance of a molecule or atom to external perturbations. It is defined as the energy required to add or remove an electron from a system and plays an important role in a wide range of chemical and physical phenomena. As a periodic descriptor, chemical hardness has the potential to be used for predicting the chemical and physical properties of materials, including their reactivity, solubility, and stability. The concept of chemical hardness was first introduced by Pearson in 1963, who proposed the principle of hard and soft acids and bases (HSAB) to explain chemical reactions between acids and bases. Since then, chemical hardness has been extensively studied, and it has become a powerful tool in the development of new materials and compounds. This article provides an overview of chemical hardness as a periodic descriptor and its potential applications in chemistry and materials science.

REVIEW OF RELATED LITERATURE

In 2016, Giri et al. published a study in which they used DFT calculations to investigate the chemical hardness of transition metal carbides. They found that the chemical hardness of these materials is closely related to their electronic structure, and that doping with certain elements can significantly increase their chemical hardness.

In **2017, Bhowmik et al.** published a study in which they used DFT calculations to investigate the chemical hardness of lithium-ion battery cathode materials. They found that the chemical hardness of these materials is closely related to their intercalation potential, and that materials with higher chemical hardness are more resistant to degradation during battery cycling.

In **2018, Sarkar et al**. published a study in which they used DFT calculations to investigate the effect of alloying on the chemical hardness of aluminum-based materials. They found that the chemical hardness of these materials can be significantly increased by alloying with certain elements, and that this can lead to improved mechanical properties and wear resistance.

In **2019, Gupta et al.** published a study in which they used DFT calculations to investigate the chemical hardness of metal-organic frameworks (MOFs). They found that the chemical hardness of MOFs is closely related to their porosity and surface area, and that this can be used to design new MOFs with specific properties for applications in gas storage and separation.

In **2020, Bhattacharyya et al.** published a study in which they used DFT calculations to investigate the chemical hardness of layered transition metal dichalcogenides. They found that the chemical hardness of these materials is closely related to their electronic structure and that doping with certain elements can significantly increase their chemical hardness, making them potentially useful materials for applications in catalysis and energy storage.

COMPUTATIONAL METHODS

It is well known that electronegativity and atomic stiffness descriptors describe the same underlying structure and origin. They rely on the valence electrons' ability tattract other electrons . The exact relative values of electronegativity and stiffness, i.e $\chi \alpha \eta$, were also stated by Putz, M. V. et al. There is no statistical or physical change when electronegativity is added to atomic stiffness, as demonstrated by Ghosh, D. C. et al..

The current system established a brand unique scale with an atomic hardness of one hundred three elements of the periodic table in relations of force idea. Allred, A. L. et al. first advocated a range of electronegativity focused on electrostatic intensity applying the following ansatz:

$$\chi \alpha Z_{eff} \frac{e^2}{r^2} \qquad (1)$$

In all cases where χ takes the form of electronegativity, r still represents the gap between an electron's nucleus and its outermost shell. The nucleus and the surrounding electrons cause the electron to retain its charge even after Zeff has removed it. The electron is protected from the nuclear charge Z by a shield, hence the more accurate phrase Z_{eff}.

If we assume that the electronegativity of a molecule is equal to its hardness, we can propose a new ansatz, which is as follows:

$$\eta \alpha Z_{eff} \frac{e^2}{r^2} \qquad (2)$$

The Principle of Hardness Equivalence

The principle of electronegativity equality (EEP) is a well-established empirical law. Sanderson, R. T. created this essential notion in 1951 to explain how chemical bonds are formed. Many further findings are reported on this phenomena . Hardness, like electronegativity, is an important periodic descriptor with a similar basis of construction. The principle of hardness equalisation has been the subject of a small number of studies . According to the hardness equalisation principle, the hardness kernel's magnitude varies as a result of the chemical reactions that form bonds. When atomic hardness is normalized, the range of atomic particle hardness standards will correct to a handful of midway values , i.e.

$$\eta_{AB} = \eta_A^{*} = \eta_B^{*} \qquad (3)$$

Where, η_A^{*} and η_B^{*} are the hardness.

It is widely known that the normalised molecular hardness can be calculated by using the geometric mean of the atomic hardness .

$$\eta_{GM} = \sqrt{\eta_A \cdot \eta_B}; \text{Where } \eta_{GM} \text{ is reported for molecular hardness} \qquad (4)$$

RESULTS AND DISCUSSION

In the context of power theory, this is the first attempt to calculate atomic stiffness. In Table-1, we provide the results of our calculations using the force concept for the atomic hardness of following elements.

Table 1 Chemical hardness of Elements

Symbols of Element	Hardness (ɳ) Calculated	Atomic Number	Symbols of Element	Hardness (ɳ) Calculated
H	5.96	52	Te	10.27
He	46.32	53	I	15.57
Li	0.69	54	Xe	23.58
Be	3.50	55	Cs	0.56
B	3.43	56	Ba	1.34
C	8.43	57	La	1.88
N	18.17	58	Ce	2.12
O	17.81	59	Pr	2.39
F	36.44	60	Nd	2.78
Ne	68.44	61	Pm	3.18
Na	1.02	62	Sm	3.61
Mg	3.10	63	Eu	4.00
Al	2.19	64	Gd	5.16
Si	5.05	65	Tb	5.02
P	10.18	66	Dy	5.54
S	11.15	67	Ho	6.11
Cl	20.71	68	Er	6.69

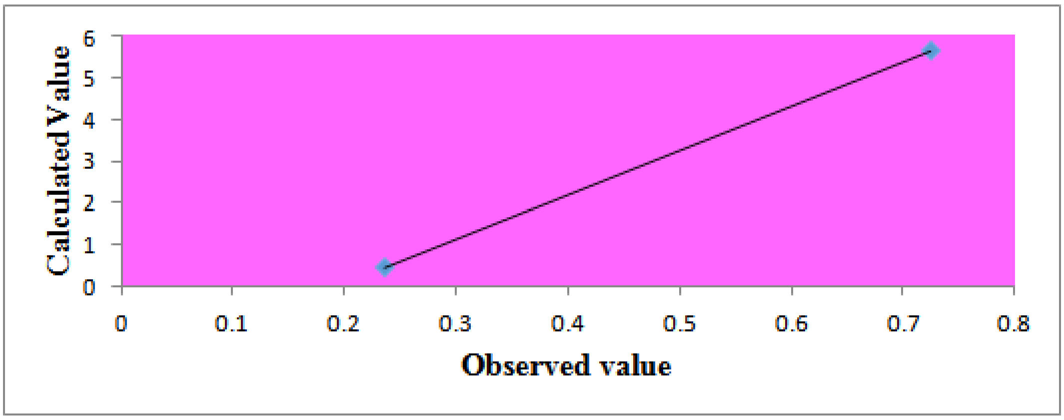

Figure 1: Observed value set against the calculated value of hardness forAtomic Number 1-2

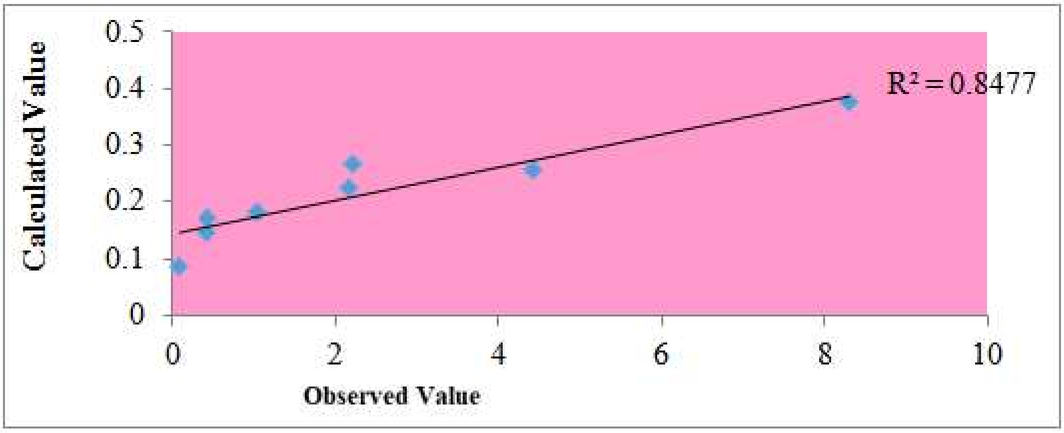

Fig. 2 Observed value set against the calculated value of hardness forAtomic Number 3-10

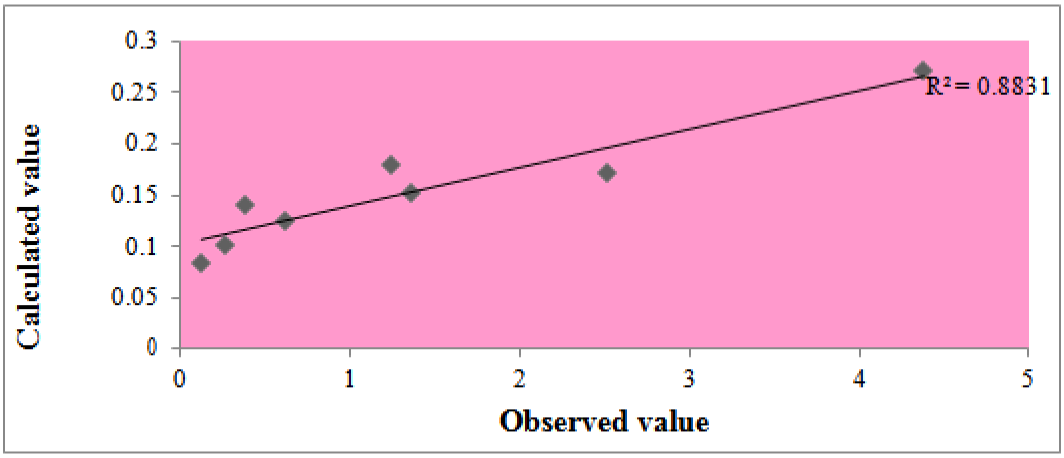

Figure 3 Observed value set against the calculated value of hardness forAtomic Number 11-18.

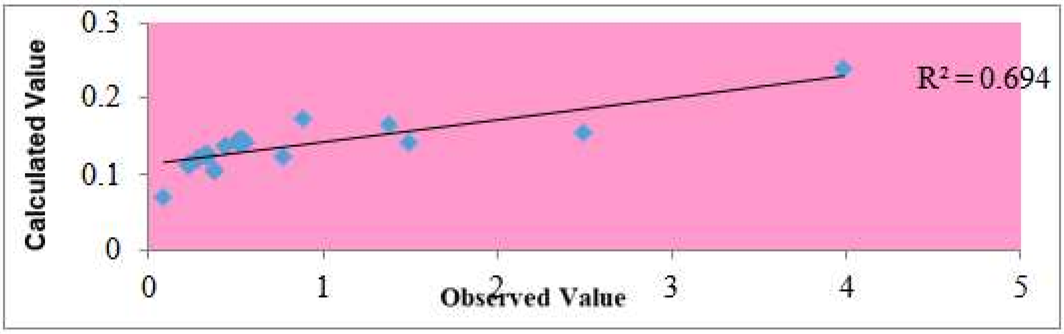

Figure 4 Observed value set against the calculated value of hardness forAtomic Number 19-36

Table 2 Values of constant a and b Period wise in the Period table

Period	a	b
1	10.57	2.035
2	0.033	0.138
3	0.037	0.102

4	0.029	0.112
5	0.038	0.105
6s	-20.83	1.586
6 Lanthanide	0.018	0.095
6 Transition elements	0.016	0.123
7s	34.78	-2.55
7 Actinide	0.022	0.098

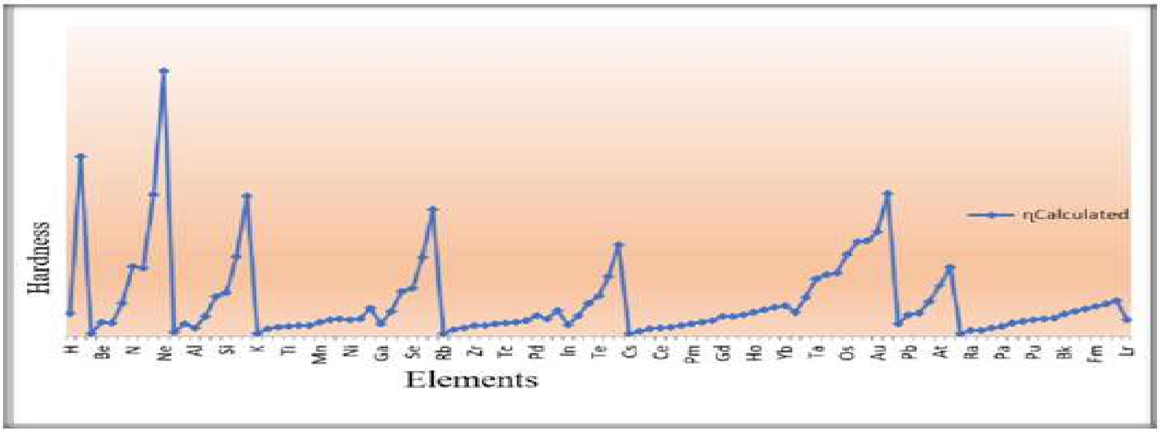

Figure 5: Calculated hardness of one hundred three elements of the periodictable in terms of atomic number.

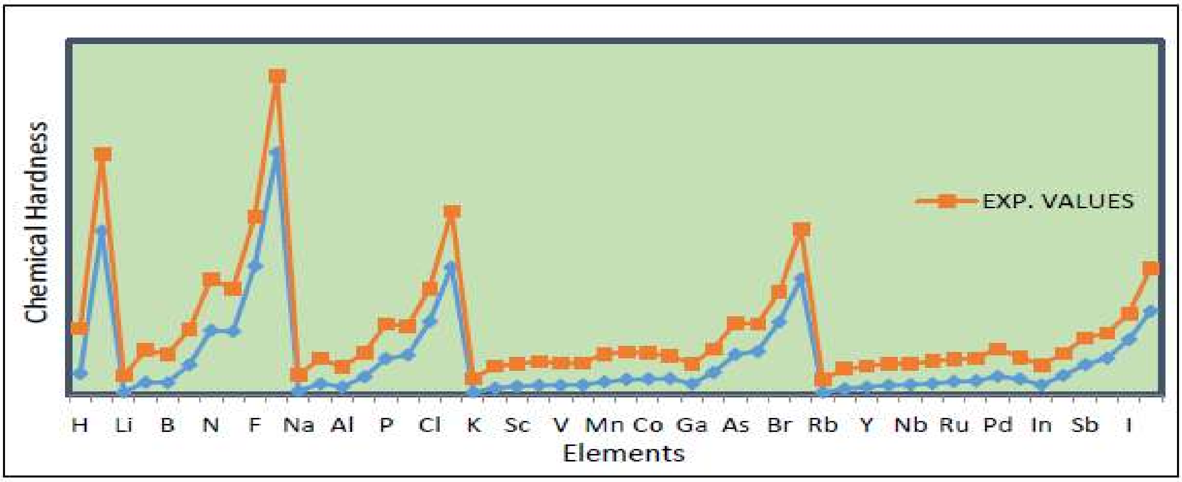

Fig. 6: Comparative Analysis of Computed Elemental hardness *vis-a-vis* Experimental values

Table 3: Different Observed Values and computed hardness of Some Elements

Atomic No.	Symbols of Element	η (Calculated)	η(eV)	η(Pearson)	η(Putz)	η(RB)
1	H	5.96	6.43	6.43	6.45	6.83
2	He	46.32	12.54		25.79	16.88
3	Li	0.69	2.37	2.39	0.65	3.06
4	Be	3.50	3.50	4.5	1.69	5.16
5	B	3.43	4.62	4.01	3.46	4.39
6	C	8.43	5.74	5	6.21	5.49
7	N	18.17	6.86	7.23	9.59	8.59
8	O	17.81	7.99	6.08	13.27	6.42
9	F	36.44	9.11	7.01	16.16	7.52
10	Ne	68.44	10.23		17.87	15.45
11	Na	1.02	2.44	2.3	0.66	2.91
12	Mg	3.10	3.01	3.9	0.93	4.63
13	Al	2.19	3.58	2.77	1.42	2.94
14	Si	5.05	4.16	3.38	2.1	3.61
15	P	10.18	4.73	4.88	2.92	5.42
16	Si	11.15	5.30	4.14	3.82	4.28
17	Cl	20.71	5.87	4.68	5.01	4.91

Since hardness is a periodic attribute, we cannot determine it by solving the Schrödinger equation because there is no quantum mechanical operator to do so. In this process, we have employed a simple theoretical way to determine the hardness of individual atoms. Hardness is lowest for alkaline elements and highest for noble ones. IE and hardness plots are quite congruent. The value of hardness equalisation agrees perfectly with hardness data obtained through experimentation. All the requisites for the full atomic hardness scale are met by our processed data. Both partial and complete shell layouts are acknowledged. In our calculation, the relativistic effect is very noticeable. The notion of hardness equalisation can be applied to our data with confidence.

FUTURE SCOPE

Chemical hardness is a fundamental concept in the field of theoretical and computational chemistry that describes the resistance of a molecule or atom to external perturbations. It is defined as the energy required to add or remove an electron from a system, and it plays an important role in a wide range of chemical and physical phenomena.

As a periodic descriptor, chemical hardness has the potential to be used for predicting the chemical and physical properties of materials, including their reactivity, solubility, and stability. The future scope of chemical hardness as a periodic descriptor is vast, and it is likely to play an increasingly important role in the development of new materials and compounds with desired properties. One potential application of chemical hardness is in the design of new catalysts for chemical reactions. By understanding the chemical hardness of different catalysts, researchers can develop more efficient and effective catalysts for specific reactions, leading to the development of new materials and technologies.Chemical hardness can also be used to predict the behavior of molecules in different environments, such as in solution or at interfaces. By understanding the chemical hardness of different molecules, researchers can design materials that are better suited for specific environments, leading to more efficient and effective chemical processes.

In addition, chemical hardness can be used to study the properties of materials under extreme conditions, such as high pressure or temperature. By understanding the chemical hardness of materials under these conditions, researchers can develop new materials that are better suited for these environments, leading to new technologies and applications.

CONCLUSION

Any proposed theory needs to be able to account for existing experimental data in order to gain acceptance. The strength of an atom is not something that can be measured experimentally or even calculated to a substantial degree. Establishing a new absolute hardness scale in the absence of a small number of experimental standards depends on the periodic behaviour of hardness. There have been comparisons made to existing scales and real-world applications. For this endeavor, we need to suggest an ansatz to compute global hardness of element in relations of force model based on substantial connection between atomic hardness of particles and atomic radii.

One hundred and three elements from the periodic table have had their chemical hardness determined using our proposed ansatz. The complete sine qua non of repeatable performance can be attributed to computed data. The differences between the half-filled and full-filled shell structures are defined. Our model is supported by the results of a comparison analysis with established hardness scales. Our computed hardness data has been used to construct the Hardness Equalisation Principle. We find good agreement between the equalisation molecular hardness we calculate and that found in experiments.

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