INTERNATIONAL JOURNAL
FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Electronegativity: A Mnemonic Number Code for an Atom

P. Ramakrishnan

Chemical Engineering Department, National Institute of Technology, Rourkela, Odisha – 769008, India

Abstract: An attempt is made to substantiate that, electronegativity expressed as Hellman-Feynman force(Force by Nucleus on electron) or Ehrenfest force(Force by electron on Nucleus) will be accurate and absolute. The concept of Hellman-Feynman force as an equivalence of Born-Oppenheimer approximated energy for di-atomic system and Hartree-Fock force as an equivalence of Hartree-Fock approximated energy for polyatomic system have been critically analyzed. An extended theory of Electronegativity based on Force concept is established. Electronegativity values computed for various elements using Hellmann-Feynman force exerted on the nuclei and the Ehrenfest force exerted on the electron density are presented.

I. INTRODUCTION

All models of electronegativity are theorized by individual's intuition. The qualitative understanding of electronegativity is not up to the mark. Universal acceptance on the common agreement of the all models till to 2019 A.D seems impossible. Force model of electronegativity was defined first by AL Allred and EG Rochow[1] with help of electrostatic field. According to this definition, electronegativity is equal to Coulomb force of attraction between the nucleus and an electron at the covalent radius.

$$c_{AR} \,^\circ\, Z^* \frac{e^2}{r^2} \tag{1}$$

Where $Z^* = Z - \sigma$, r is covalent radius for the atom(considering smaller value as well as outer radial maxima). The Coulomb force is a measure of power of an atom in a molecule that drags electron towards nucleus. Therefore, electronegativity is an absolute one. c_{AR} dimension is not straight forward as it is evaluated through eq. 1. The quantity Z^*/r^2 was calculated through Pauling's work and Slater rules[2,3]. Pauling's Scale and Allred-Rochow scale can be made to coincide by expressing the electronegativity from the electrostatic approach as the linear function of Z^*/r^2. Here mean radius is expressed in picometer.

$$\chi_{AR} \equiv 3590(z*/r2) + 0.744 \qquad \text{EQ (2)} \quad \text{WHERE } 3590 \text{ AND } 0.744 \text{ ARE NUMERICAL CONSTANTS.}$$

Introduction of the idea of force into electronegativity theory makes this scale seem quite consistent with Pauling's definition. It also emphasizes the idea for simple calculation, because r and Z^* are readily available quantities for many elements. It is to be noted that, this scale independent of electron affinities and bond dissociation energies. Slater rules for finding effective nuclear charge are empirical.

Four extension of the Allred and Rochow's idea were reported by different authors. The first extension of Allred-Rochow scale by Huhee[4] is based on two assumptions, r of order $(1/Z^*)$ and Z^* of order σ.

$$c_H = 0.36 \,´\, \frac{(Z^* - 3s)}{r^2} + 0.74 \tag{3}$$

The second extension of Allred-Rochow scale by Boyd and Markus[5] is based on non empirical approach. The empirical covalent radius is replaced by relative covalent radius obtained from the free atom wave function by density contour technique. The effective nuclear charge is obtained through integration of radial density function from nucleus to relative distance. Electrostatic electronegativity is expressed as,

$$c = \frac{Z}{r^2} \left[1 - \int_0^r r(r)dr \right] \tag{4}$$

The radial charge density $\rho(r)$ can be obtained from the Hartree Fock atomic orbitals data[113], [114]. The computed electronegativity values follow the general pattern of Mulliken ground state electronegativity values with an exception for groups 2 and 3 of periodic table because $\rho(r)$ decreases as per the expectation rule i.e. $\langle IP' \ r \rangle > ¥$.

The third extension of the scale was made Mande et al. [6] where the value of effective nuclear (Z^*) charge was obtained spectroscopic analysis. Therefore, the values become less arbitrary than that of Slater's. This electronegativity scale is more fundamental and reliable. The correlation of the scale is excellent with that of Pauling's scale. The electronegativity values obtained for 1st transition metals are more reasonable than Allred-Rochow scale.

The fourth extension of this scale was made by Yonghe Zhang[7] where electronegativity was calculated on the basis of electrostatic force given by,

$$F = n^{*} \ ' \ \frac{\sqrt{IP_z / Ry}}{r^2} \tag{5}$$

WHERE $$IP_z = Ry \left(\frac{Z^*}{n^*} \right)^2 \tag{6}$$

IP_Z is ultimate ionization potential for outer electron. This type of scale is based on the concept of different electron attracting power of an element in different valence state. Therefore, electronegativity is termed as a function of oxidation number. Zhang has also reported dual parameter equation[12]. Zhang electronegativity is given by,

$$c_z = 0.241F + 0.775 \tag{7}$$

$$Z = \frac{Z}{r_i^2} - 7.7c_z + 8.0 \tag{8}$$

In this section, an independent approach to define electronegativity is presented. The force expression based on Hellmann-Feynman theorem is proposed as electronegativity. Moreover, this force must be equivalent to the primary definition of electronegativity such as ability of an atom to attract electron towards itself. Following the proposition, the definition of electronegativity becomes 'inherent ability of an atom to attract and hold electron'. The electronegativity in terms of Hellmann Feynman force is equal to Born Oppenheimer force for an atom in diatomic system and Hartree -Fock force of an atom in poly atomic system. Prior to the force based definition of electronegativity and relevant correlations, the four relevant force concepts are briefly discussed. Born-Oppenheimer Force within the Born-Oppenheimer approximation is expressed as a balance of two opposing terms such as one from Nuclear-Nuclear repulsions and other from Electron-Nuclear attraction. The latter is conceived as the 3-D electron density.This force concept arises out of Born Oppenheimer(BO) energy approximation. M Born and J R Oppenheimer[8], [9] have contributed a celebrated paper to science. It brings the systematic correspondence of the energy of electronic motion, nuclear vibration and rotation to the terms of power series in the fourth root of electron nucleus mass ratio. Born and Oppenheimer suggested that total wave function (y) can be written as the product of the nuclear wave function (y_n) and electronic wave function (y_e). This approximation simplifies complicated Schrödinger equation into electronic equation ($H_e y_e = E_e y_e$) and nuclear equation ($H_n y_n = E_e y_e$). The equation devised by them for the rotation represents a generalization of the treatment of Kramers theorem and Pauli exclusion principle. This approximation also justifies Frank-Condon principle used in explaining the intensity of band lines. In the last several decades, rigorous mathematical work has been reported on the validity of the BO approximation. Quite a few number of papers contain the study of BO have reported that, a reduced Hamiltonian is an appreciable approximation to true molecular HamiltonianHowever, a few of those are closely related to works on semi classical Schrodinger matrix operators[10-26]. BO approximation is based on "assumption of ignoring motions of nearly stationary nuclei with much larger mass and smaller velocity with respect to motion of electron with much smaller mass and larger velocity". The approximation holds good for the ground state of molecule and breaks down for the excited state. Complete Hamiltonian is represented as

$$H = H_n + \ H_e = T_n + \ T_e + \ V_{nn} + \ V_{en} + \ V_{ee} \tag{9}$$

$$H = -\frac{1}{2}\sum_A \tilde{N}_A^2 - \frac{1}{2}\sum_i \tilde{N}_i^2 + \sum_{B,A}\frac{Z_A Z_B}{|R_B - R_A|} - \sum_{A,i}\frac{Z_A}{|r_i - R_A|} + \sum_{i,j}\frac{1}{|r_i - r_j|} \qquad \textbf{10}$$

Again, Molecular Hamiltonian (H^{mol})

$$H^{mol} = -\frac{1}{2}\sum_A \tilde{N}_A^2 - \frac{1}{2}\sum_i \tilde{N}_i^2 + \sum_{B,A}\frac{l^2 Z_A Z_B}{|R_B - R_A|} - \sum_{A,i}\frac{l\, Z_A}{|r_i - R_A|} + \sum_{i,j}\frac{1}{|r_i - r_j|} \quad \textbf{11}$$

λ is treated as parameter and it may vary between 0 and 1. The exact solution to the electronic Schrodinger equation, obtained from BO approximation can be reachable for one electron systems.

II. HARTREE-FOCK FORCE

This force concept arises out of Hartree-Fock energy approximation for multi electronic systems. The Hartree-Fock approximation is a good enough to approximate the energies and wave function. The electronic Hamiltonian and energy based on Hartree-Fock approximation can be written as follows .

$$H_e = \sum_i z(a) + \sum_{a<b} h(a,b) + V_{nn} \qquad \textbf{12}$$

The first term represents a one electron operator, the second term represents a two electron operator and third term is a constant for the fixed set of nuclear coordinates

$$E_{hf} = \sum_a \langle a|z|b\rangle + \frac{1}{2}\sum_{ab}([aa|bb] - [ab|ba]) \qquad \textbf{13}$$

Where the first term represents one electron integral, the second term represents two electron Coulomb integral, the third term represents exchange integral. All the integrals can be computed by existing computer algorithms. The energy difference between non relativistic energy of the system and Hartree-Fock limit energy is considered as both static and dynamic electronic correlation energy. The derivative ($-\partial H_e / \partial V$) of electronic Hamiltonian operator w.r.t. distance of nucleus of an atom from electron can also be defined in quantum mechanics and also this represents the force on atom A due to electrons. Furthermore, within simple Born-Oppenheimer approximation and Hartree-Fock approximation, Energy (E) plays the role of potential energy for actual motion. Moreover, $\partial E / \partial V$ replaces the above derivative and it is equal to the BO force (also Hartree Fock force) because nuclear coordinates are simply treated as external parameters.. This force is better to be termed as BO force in the steady state. The electronegativity will be equal to B-O force (also Hartree Fock force).

III. HELLMAN-FEYNMAN FORCE

The force concept is the consequence of Hellmann Feynma theorem .The expression for this theorem have already been reported by different authors[27]–[38]. This concept dictates that the actual force on any nucleus can be interpreted in terms of classical electrostatics if three dimensional charge distribution in a system of electrons and nuclei were known from quantum mechanical procedure. The force on a nucleus will be equal to charge on that nucleus times the electric field due to all electrons and other nuclei. R Feynman further stated that a three dimensional electron cloud in a molecule is restricted from collapsing as it obeys Schrödinger equation. The force concept explains the nature of chemical bonding, the change in molecular shape on excitation and chemical reaction. Energy concept is not proved to be satisfactory always because they lack the simplicity and elegant nature. A.C.Hurley[36]–[38] has given the theoretical justification of the actual use of such electrostatic approach and shown that the force calculations are valid even for approximate wave functions. The Hellmann Feynman force concept have been used (i) by R.F.W.Bader[39]–[43] for interpreting chemical binding, (ii)by Koga T and H.Nakatsuji[44]–[46] for force modelling of molecular geometry,(iii)by P.Politzer and K.C.Daiker[47], [48] for models of Chemical Reactivity, (iv) by A.J.Coleman[49]–[51] for calculation of first and second order reduced density matrices. It also withstands the critical examination of theoretical physists and chemists as well. This force concept has certain advantage over the concept of total energy even though the calculation of force

always involves an approximate charge density function. The advantage of calculating charge density is possible through molecular orbital method. The total force on a nucleus is simple sum of orbital contributions but total energy is not sum of orbital energies. The second advantage is that, force is an expectation value of one electron, momentum independent operator. It is more sensitive to any change in wave functions than energy. T Berlin[52] gave clear interpretation of this electrostatic force arising out of Hellmann Feynman theorem. This force is equivalent to infinitesimal change in energy per change in distance (parameter). Classical physics states that, a force is the negative gradient of energy. He proposed a term binding (related force acting on the nucleus) in place of bonding (related to changes in energy) in the picture of chemical bonding. He has proposed the physical partitioning of three dimensional space of electrons of diatomic system into a binding region ($f_i > 1$), anti-binding region($f_i < 1$) and the nonbinding region($f_i = 1$) . The charge density is positive everywhere and thus the sign of contribution to force to the charge in each volume element depends on the sign of f_i. The net value of f_i around 1 helps to assign the electronegativity to the concerned atom in molecule for the diatomic system with $Z_B > Z_A$, the anti-binding region for A is closed while anti-binding region for B in the limit $Z_B >> Z_A$ approaches a plane perpendicular to inter nuclear axis. The idea of closing of anti-binding region is used to justify to assign more electronegativity value to B. Hellmann Feynman force equation can be written in various forms. At static equilibrium geometry, Hellman Feynman force is zero but at dynamical equilibrium geometry, this force can never be equal to zero for which the magnitude of Hellman Feynman force is reasonably to be construed as power of nucleus of an atom to attract electron towards itself.

GENERALIZED FORM OF HELLMAN FEYNMAN FORCE FOR BOTH STEADY STATE AND NON- STEADY STATE IS REPRESENTED AS,

$$F_V = F_V = - \partial E / \partial V = - \int \psi \psi^* (\partial H_e / \partial V) dv \qquad \text{EQ 14}$$

$$- \frac{\partial E}{\partial V_A} = - \sum_{B,A} \frac{Z_A Z_B}{|R_B - R_A|^2} + \int \frac{Z_A}{|r_i - R_A|^2} r(r) dr \qquad \text{EQ 15}$$

Where the first term is independent of the electronic coordinates and is constant during integration over the coordinates. This term gives ordinary columbic force of repulsion between the nuclei. The second term represents charge density distribution due to ith electron.

$$- \frac{\partial E}{\partial V_A} = - 2l \sum_{B,A} \frac{Z_A Z_B}{|R_B - R_A|} + \sum_A Z_A \int \frac{r(r,l)}{|r_i - R_A|} dr \qquad 16$$

Where the λ is a parameter which solves two problems. Firstly, it helps to apply simultaneously to all nuclei. Secondly it is a continuous function between 0 and 1 so that differentiation of energy w.r.t. nuclear coordinates is made possible.

The other form of Hellmann-Feynman force equation can be written as

$$F_z = \frac{Z_A}{R_A^2} \left[Z_B - \sum_i f_i(R_A) \right] \qquad 17$$

$$= - \frac{1}{2} \int f(r) r(r) dr \quad \text{WHICH IS ELECTRONIC CONTRIBUTION TO THE FORCE ON EITHER NUCLEUS}$$

The term f(r) is called berlin quantity[52]. And also the electronic contribution in terms of the quantum mechanical average of the electric field operator is also mathematically represented as,

$$F_z = Z_A \int dr .... \int \psi^* \left[\sum_{i=1}^n \tilde{N}_A (|r_i - R_A|)^{-1} \right] \psi \, dr_n \qquad \text{EQ.18}$$

The equivalence of the electron in the above equation is equivalent to n times the average force exerted on an atom by one electron so the above equation can be written in the form of electronic charge density.

$$F_z = Z_A \oint \tilde{N}_A \left(|r - R_A| \right)^{-1} r(r) dr \qquad \text{EQ. 19}$$

Where, $r(r) = n \oint ds_1 \oint dx_2 ... \oint y^*_{(x_1, x_2, ..., x_n)} y_{(x_1, x_2, ..., x_n)} dx_n$ Eq.20   Where ρ(r) denotes

electronic charge density in a stationary state, ρ(r) dr stands for amount of electronic charge in a volume element dv and x_i denotes the product of space co-ordinate (r_i) and spin co-ordinate(s_i) of the ith electron. The interpretation of ρ(r) as a physical model of the electrons in line with the HF theorem includes the possibility of ascribing a value to the electrostatic force exerted at atom A by each and every element ρ(r) dr.

IV. EHRENFEST FORCE

The Ehrenfest force theorem, a primal force theorem involves fluxes of corresponding current density through the surface bounding the system whether this be a surface of zero-flux for an atom in a molecule or the surface bounding an infinitesimal volume element, the properties of which are described in the local form of the theorem. The atomic statement of Ehrenfest force is given as,

$$m \int_{(A)} dr \partial j(r) / \partial t = \int_A dr \int dr' \psi * (-\nabla \hat{V}) \psi + \oiint dS(r_s) . \sigma_s(r) \quad ....21$$

sity at the point r and the left side integral in the above expression represents the rate of change of the total momentum of electron density in atomic-basin(A).The first term in the right side integral not only comes from averaging of the commutator

$\prec i / (h / 2\pi) \succ [H.P]$ but also represents the Ehrenfest force, $F(r,t) = N \int dr' \psi * < -\nabla V' > \psi$ ......

..........................22

where $\nabla \hat{V}$ is the gradient with respect to coordinates of electron located at r of total potential energy operator $\hat{V}$ which speaks of all interactions within the system and $-\nabla \hat{V}$ is the force exerted on the electron at position r by all of remaining electrons and nuclei in the system.And also the net force exerted on the electron density distribution r(r) in a molecule at point r, i.e. the sum of the attraction forces by all the nuclei and repulsion forces by the average electron density, is the Ehrenfest force.

A. Scientific Justification for correlation among Electronegativity, Hellman-Feynma & Ehrenfest Force

The Hellmann Feynman electrostatic force leads two opposing terms, one from nuclear nuclear repulsions and other from electron nuclear attractions.

The electron-nuclear attractive force is expressed in terms of three dimensional electron density. This force can be termed as charge equivalent force. This follows from the energy approximations postulated by Born Oppenheimer for di atomic system and Hartree Fock for poly atomic systems.

This is true as, the fast motion of electron allows electronic wave function and probability density for immediate adjustment to changes in nuclear configuration. The fast motion of electron causes the sluggish nuclei to see electrons as charge cloud rather than discrete particles.

This fact affirms the force as electrostatic by nature thereby ruling out the possibility of mysterious quantum mechanical force in mono atomic, di atomic as well as poly atomic systems.

Electronegativity of an atom (A) just in a bonding molecule AB may be defined as Hellmann Feynman force exerted on atom (A) due to electron. The state of molecule is conceived as dynamical equilibrium geometry where Hellman-Feynman force can never be zero but at static equilibrium geometry, this force becomes zero. The first definition of electronegativity i.e. "the power of an atom to attract electron towards itself" is construed as Hellmann-Feynman Force.

This is also equivalent to Hartree Fock force in steady and non-steady states. In steady state, $r(r)$ may be interpreted as a number or charge density and $r(r)dr$ as amount of electronic charge in the volume element. Based on above explanation, Electronegativity=Hellmann-Feynman Force=Ehrenfest Force.

$$c = F_{VA} = F(r,t) \quad ....23$$

Based on the BO approximation

$$F_{VA} = - \frac{\P E}{\P V_A} = - \sum_{B,A} \frac{Z_A Z_B}{|R_B - R_A|^2} + \oint \frac{Z_A}{|r_i - R_A|^2} r(r) dr \qquad 24$$

Based on the basis of Hartree-Fock approximation

$$F_{VA} = - \frac{\P E}{\P V_A} = - 2l \sum_{B,A} \frac{Z_A Z_B}{|R_B - R_A|} + \sum_A Z_A \oint \frac{r(r,l)}{|r_i - R_A|} dr \qquad 25$$

First terms in eq. 24 and 25 represent classical nuclear contribution. Second terms in eq. 24 and 25 above represent electronic contribution.

V.   COMPUTATION OF ELECTRONEGATIVITY AND DISCUSSION

Electronegativity in terms of energy gradient in au/picometer unit.

A. $c_{E-\ slater} = \dfrac{E_{hf}}{r_{slater}}$ 　　　　　　26

B. $c_{E-\ clementi} = \dfrac{E_{hf}}{r_{clementi}}$ 　　　　　　2

C. $c_{E-\ absolute} = \dfrac{E_{hf}}{r_{absolute}}$ 　　　　　　28

Electronegativity in terms Coulomb force.

D. $c_{f-\ slater} = \dfrac{Z^*_{slater}}{r^2_{slater}} \times 1000$ 　　　　　　2

E. $c_{f-\ clementi} = \dfrac{Z^*_{clementi}}{r^2_{clementi}} \times 1000$ 　　　　　　30

F. $c_{f-\ absolute} = \dfrac{Z^*_{clementi}}{r^2_{absolute}} \times 1000$ 　　　　　　31

FOR REFERENCE, 1 au of force $= \left(\dfrac{e}{a_0} \right)^2$

In eq.29-31, 1000 is multiplied to make the data more convincible. Electronegativity values based on energy and force from Hydrogen to Lawrencium have been computed through the above equations and are mentioned in table 1 and 2. In case of unavailability of data the spaces are '*' marked.

The necessary data for Hartree-Fock Energy[53], Z* Slater effective nuclear charge[54], Z* Clementi effective nuclear charge[57]-[58] ,Density-metric radius[59] Absolute Radius[60] and calculated Clementi Radius[57]- [58] and are taken from cited references.

Table 1. Electronegativity Data based on Hartree Fock Energy equivalence of Hellmann-Feynman Force

Element Symbol	E_{hf} (au)	r_{slater} (pm)	r_{clemen} (pm)	$r_{absolute}$ (pm)	$c_{e\text{- slater}}$	$c_{e\text{- clementi}}$	$c_{e\text{- absolute}}$
H	0.49994557	25	53	52.92	0.019998	0.009433	0.009447195
He	2.86115334	120	31	31.13	0.023843	0.092295	0.091909841
Li	7.43271968	145	167	162.83	0.05126	0.044507	0.045647115
Be	14.5729681	105	112	108.55	0.13879	0.130116	0.134251203
B	24.4144654	85	87	81.41	0.287229	0.280626	0.299895165
C	37.5310547	70	67	65.13	0.536158	0.560165	0.576248345
N	54.4042654	65	56	54.28	0.836989	0.971505	1.00228934
O	74.6191049	60	48	46.52	1.243652	1.554565	1.604022031
F	99.1639672	50	42	40.71	1.983279	2.361047	2.435862619
Ne	128.546472	160	38	36.71	0.803415	3.382802	3.50167453
Na	161.8586	180	190	216.5	0.899214	0.851887	0.747614781
Mg	199.614215	150	145	167.11	1.330761	1.37665	1.194507899
Al	241.802199	125	118	136.08	1.934418	2.049171	1.776912103
Si	288.757442	110	111	114.77	2.625068	2.601418	2.515966211
P	340.718822	100	98	99.22	3.407188	3.476723	3.433973211
S	397.384664	100	88	87.39	3.973847	4.515735	4.547255567
Cl	459.338687	100	79	78.08	4.593387	5.814414	5.882923758
Ar	526.816781	71	71	70.56	7.419955	7.419955	7.466224221
K	599.164348	220	243	329.3	2.723474	2.465697	1.819509104
Ca	676.757668	180	194	254.19	3.759765	3.488442	2.662408702
Sc	759.553865	160	184	241.49	4.747212	4.12801	3.145280819
Ti	848.05445	140	176	329.98	6.057532	4.818491	2.570017728
V	942.482641	135	171	219.53	6.981353	5.511594	4.293183806
Cr	1043.35589	140	166	210	7.452542	6.285276	4.968361381
Mn	1149.86888	140	161	201.24	8.213349	7.142043	5.713918108
Fe	1262.18252	140	156	193.19	9.015589	8.090914	6.533373984
Co	1380.93099	135	152	185.75	10.22912	9.085072	7.434352571
Ni	1506.33054	135	149	178.88	11.158	10.1096	8.420899709
Cu	1638.96277	135	145	172.5	12.14046	11.30319	9.501233449
Zn	1777.84664	135	142	166.54	13.16923	12.52005	10.67519299
Ga	1923.18595	130	136	144.89	14.79374	14.14107	13.27342087
Ge	2075.26686	125	125	128.23	16.60213	16.60213	16.18394182
As	2234.23911	115	114	114.5	19.42817	19.59859	19.51300533
Se	2399.75947	115	103	104.24	20.86747	23.29864	23.02148379
Br	2572.31642	115	94	95.32	22.36797	27.36507	26.98611435
Kr	2752.05419	*	88	87.82	*	31.27334	31.33744238
Rb	2938.35681	235	265	384.87	12.50365	11.08814	7.634673552
Sr	3131.545	200	219	297.09	15.65773	14.29929	10.5407284
Y	3331.55545	180	212	282.44	18.50864	15.71488	11.7956219
Zr	3538.75135	155	206	268.8	22.83065	17.1784	13.16499758
Nb	3753.43518	145	198	256.58	25.88576	18.95674	14.62871299
Mo	3975.55206	145	190	254.43	27.4176	20.92396	15.62532744
Tc	4204.79397	135	183	235.2	31.14662	22.97702	17.87752538
Ru	4441.23215	130	178	225.79	34.16332	24.95074	19.66974689
Rh	4685.53924	135	173	217.11	34.7077	27.08404	21.58140684

Pd	4937.9198	140	169	209.07	35.27086	29.21846	23.61850002
Ag	5197.69786	160	165	201.6	32.48561	31.5012	25.78223145
Cd	5465.1321	155	161	194.65	35.25892	33.94492	28.07671256
In	5740.10075	155	156	169.34	37.03291	36.79552	33.89689825
Sn	6022.84999	145	145	149.86	41.5369	41.5369	40.18984379
Sb	6313.48607	145	133	134.4	43.54128	47.46982	46.97534278
Te	6611.69122	140	123	121.83	47.22637	53.75359	54.2698122
I	6917.8755	140	115	111.41	49.4134	60.15544	62.09384705
Xe	7232.13748	*	108	102.63	*	66.96424	70.4680647
Cs	7553.93311	260	298	424.33	29.05359	25.34877	17.80202463
Ba	7883.54325	215	253	327.53	36.66764	31.16025	24.06968293
La	8220.95071	195	195	266.73	42.15872	42.15872	30.82124512
Ce	8566.37167	185	158	224.94	46.30471	54.21754	38.08291842
Pr	8920.39371	185	247	194.47	48.21834	36.11495	45.87028184
Nd	9283.0449	185	206	171.29	50.17862	45.06332	54.1949028
Pm	9654.39094	185	205	153.03	52.1859	47.09459	63.08822414
Sm	10034.5278	185	238	138.3	54.24069	42.16188	72.55623861
Eu	10423.5496	185	231	126.15	56.34351	45.12359	82.6282172
Gd	10820.5365	180	233	115.96	60.11409	46.44007	93.31266385
Tb	11225.8464	175	225	107.3	64.14769	49.89265	104.6211221
Dy	11640.486	175	228	99.84	66.51706	51.05476	116.5914063
Ho	12064.2689	175	226	93.35	68.93868	53.38172	129.2369459
Er	12497.2944	175	226	87.65	71.41311	55.29776	142.5817958
Tm	12939.6584	175	222	82.61	73.94091	58.28675	156.6354969
Yb	13391.4548	175	222	78.12	76.5226	60.32187	171.4215924
Lu	13851.6806	175	217	74.09	79.15246	63.83263	186.9574922
Hf	14321.0157	155	208	70.56	92.39365	68.85104	202.9622406
Ta	14799.5544	145	200	67.16	102.0659	73.99777	220.3626325
W	15287.3729	135	193	64.16	113.2398	79.20919	238.2695277
Re	15784.5427	135	188	61.41	116.9225	83.96033	257.0353802
Os	16290.4713	130	185	58.9	125.3113	88.0566	276.5784601
Ir	16805.8003	135	180	56.57	124.4874	93.36556	297.0797295
Pt	17330.8587	135	177	54.43	128.3767	97.91446	318.4063696
Au	17865.3992	135	174	52.44	132.3363	102.6747	340.6826697
Hg	18408.9902	150	171	50.6	122.7266	107.6549	363.8140356
Tl	18961.7587	190	156	186.7	99.79873	121.5497	101.562714
Pb	19523.9305	180	154	165.23	108.4663	126.7788	118.1621407
Bi	20095.5875	160	143	148.18	125.5974	140.5286	135.6160582
Po	20676.4142	190	135	134.31	108.8232	153.1586	153.945456
At	21266.7841	*	127	122.83	*	167.455	173.1399829
Rn	21866.7713	*	120	131.15	*	182.2231	166.731005
Fr	22475.8581	*	*	444.79	*	*	50.53139257
Ra	23094.303	215	*	343.32	107.4154	*	67.26757253
Ac	23722.0873	195	*	326.15	121.6517	*	72.73367254
Th	24359.4372	180	*	310.61	135.3302	*	78.42451048
Pa	25006.5117	180	*	227.56	138.9251	*	109.8897508
U	25663.5826	175	*	197.67	146.649	*	129.8304376
Np	26330.6626	175	*	174.73	150.4609	*	150.6934276
Pu	27008.4196	175	*	144.96	154.3338	*	186.3163604
Am	27695.8997	175	*	129.15	158.2623	*	214.4475393

Cm	28392.6577	*	*	129.6	*	*	219.0791489
Bk	29099.5106	*	*	112.47	*	*	258.7313115
Cf	29816.6874	*	*	104.65	*	*	284.9181787
Es	30544.2078	*	*	97.85	*	*	312.1533756
Fm	31282.1408	*	*	91.88	*	*	340.4673574
Md	32030.5533	*	*	86.59	*	*	369.9105359
No	32789.5111	*	*	81.88	*	*	400.4581229
Lr	33557.611	*	*	80.86	*	*	415.008793

Table 2. Electronegativity data based on Columb Force

Element Symbol	r_{slater} pm	$r_{clement}$ pm	r_{abslou} pm	Z^*_{slater}	$Z^*_{clementi}$	$c_{f\text{-}slater}$	$c_{f\text{-}clementi}$	$c_{f\text{-}absloute}$
H	25	53	52.92	1	1	1.6	0.355	0.357
He	120	31	31.13	1.7	1.688	0.118055556	1.756	1.741
Li	145	167	162.83B\	1.3	1.279	0.061	0.045	0.048
Be	105	112	108.55	1.95	1.912	0.176	0.152	0.162
B	85	87	81.41	2.6	2.421	0.359861592	0.319857313	0.365291259
C	70	67	65.13	3.25	3.136	0.663265306	0.698596569	0.73928841
N	65	56	54.28	3.9	3.834	0.923076923	1.222576531	1.301285021
O	60	48	46.52	4.55	4.453	1.263888889	1.932725694	2.057658426
F	50	42	40.71	5.2	5.1	2.08	2.891156463	3.077286782
Ne	160	38	36.71	57.48	5.758	2.2453125	3.987534626	4.272704829
Na	180	190	216.5	2.2	2.507	0.067901235	0.069445983	0.053485805
Mg	150	145	167.11	2.85	3.308	0.126666667	0.157336504	0.118456971
Al	125	118	136.08	3.5	8.963	0.224	0.643708704	0.484021658
Si	110	111	114.77	4.15	4.117	0.342975207	0.334144956	0.312553311
P	100	98	99.22	4.8	4.903	0.48	0.510516451	0.498039109
S	100	88	87.39	5.45	5.642	0.545	0.72856405	0.738770599
Cl	100	79	78.08	6.1	6.367	0.61	1.020189072	1.04437205
Ar	71	71	70.56	6.75	7.068	1.339020036	1.402102757	1.419643821
K	220	243	329.3	2.2	3.495	0.045454545	0.059188132	0.032230253
Ca	180	194	254.19	2.85	4.398	0.087962963	0.116856202	0.068067265
Sc	160	184	241.49	3	4.632	0.1171875	0.136814745	0.079427382
Ti	140	176	329.98	3.15	4.871	0.160714286	0.157250775	0.044734531
V	135	171	219.53	3.3	4.981	0.181069959	0.170343012	0.103354356
Cr	140	166	210	3.45	5.133	0.176020408	0.186275221	0.116394558
Mn	140	161	201.24	3.6	5.283	0.183673469	0.203811581	0.130452376
Fe	140	156	193.19	3.75	5.434	0.191326531	0.223290598	0.145596304
Co	135	152	185.75	3.9	5.576	0.21399177	0.24134349	0.161608843
Ni	135	149	178.88	4.05	5.716	0.222222222	0.25746588	0.178635861
Cu	135	145	172.5	4.2	5.842	0.230452675	0.277859691	0.196328502
Zn	135	142	166.54	4.35	5.965	0.238683128	0.295824241	0.215066777
Ga	130	136	144.89	5	6.222	0.295857988	0.336397059	0.296382926
Ge	125	125	128.23	5.65	6.78	0.3616	0.43392	0.412335198
As	115	114	114.5	6.3	7.499	0.47637051	0.5770237	0.571995195
Se	115	103	104.24	6.95	8.2867	0.525519849	0.781100952	0.762628114
Br	115	94	95.32	7.6	9.028	0.574669187	1.021729289	0.993627226

Kr	*	88	87.82	8.25	9.338	*	1.205836777	1.210784922
Rb	235	265	384.87	2.2	4.985	0.03983703	0.070986116	0.033654027
Sr	200	219	297.09	2.85	6.071	0.07125	0.126582015	0.068783483
Y	180	212	282.44	3	6.256	0.092592593	0.139195443	0.078423159
Zr	155	206	268.8	3.15	6.446	0.131113424	0.151899331	0.089213745
Nb	145	198	256.58	3.3	5.921	0.156956005	0.151030507	0.089939291
Mo	145	190	254.43	3.45	6.106	0.164090369	0.169141274	0.094323556
Tc	135	183	235.2	3.6	7.227	0.197530864	0.215802204	0.13064218
Ru	130	178	225.79	3.75	6.485	0.221893491	0.20467744	0.127203943
Rh	135	173	217.11	3.9	6.64	0.21399177	0.221858398	0.140866727
Pd	140	169	209.07	4.05	6.766	0.206632653	0.236896467	0.154792015
Ag	160	165	201.6	4.2	6.756	0.1640625	0.24815427	0.166229686
Cd	155	161	194.65	4.35	8.192	0.181061394	0.31603719	0.216212664
In	155	156	169.34	5	8.413	0.208116545	0.345701841	0.29338086
Sn	145	145	149.86	5.65	10.629	0.268727705	0.505541023	0.473283049
Sb	145	133	134.4	6.3	11.617	0.299643282	0.656735825	0.643125089
Te	140	123	121.83	6.95	12.538	0.354591837	0.828739507	0.844733616
I	140	115	111.41	7.6	11.612	0.387755102	0.878034026	0.935532068
Xe	*	108	102.63	8.25	12.425	*	1.065243484	1.179635244
Cs	260	298	424.33	2.2	2.2	0.032544379	0.024773659	0.012218424
Ba	215	253	327.53	2.85	2.85	0.061654949	0.044524989	0.026567011
La	195	195	266.73	3.5	3.5	0.092044707	0.092044707	0.049195379
Ce	185	158	224.94	4.15	4.15	0.121256392	0.166239385	0.082019046
Pr	185	247	194.47	4.8	4.8	0.140248356	0.078676917	0.126921738
Nd	185	206	171.29	5.45	5.45	0.159240321	0.128428693	0.185751566
Pm	185	205	153.03	6.1	6.1	0.178232286	0.145151695	0.260481377
Sm	185	238	138.3	6.75	6.75	0.197224251	0.119165313	0.352906301
Eu	185	231	126.15	7.4	7.4	0.216216216	0.138678061	0.465004558
Gd	180	233	115.96	8.05	8.05	0.24845679	0.148280499	0.598658933
Tb	175	225	107.3	8.7	8.7	0.284081633	0.171851852	0.755648472
Dy	175	228	99.84	9.35	9.35	0.305306122	0.179863035	0.937999196
Ho	175	226	93.35	10	10	0.326530612	0.195786671	1.147549308
Er	175	226	87.65	10.65	10.65	0.347755102	0.208512804	1.386263431
Tm	175	222	82.61	11.3	11.3	0.368979592	0.229283337	1.655820287
Yb	175	222	78.12	11.95	11.95	0.390204082	0.242472202	1.958138634
Lu	175	217	74.09	12.6	12.6	0.411428571	0.267578415	2.295362888
Hf	155	208	70.56	13.25	12.6	0.551508845	0.291235207	2.530774214
Ta	145	200	67.16	13.9	13.25	0.661117717	0.33125	2.937612472
W	135	193	64.16	14.55	13.9	0.798353909	0.37316438	3.376650332
Re	135	188	61.41	15.2	14.55	0.834019204	0.411668176	3.85820055
Os	130	185	58.9	15.85	15.2	0.937869822	0.444119795	4.381400953
Ir	135	180	56.57	16.5	15.85	0.905349794	0.489197531	4.952869772
Pt	135	177	54.43	17.15	16.5	0.941015089	0.526668582	5.569385446
Au	135	174	52.44	17.8	17.15	0.976680384	0.566455278	6.236468863
Hg	150	171	50.6	18.45	17.8	0.82	0.608734311	6.952147354
Tl	190	156	186.7	5	18.45	0.138504155	0.758136095	0.529307118
Pb	180	154	165.23	5.65	5	0.174382716	0.210828133	0.183143791
Bi	160	143	148.18	6.3	5.65	0.24609375	0.276297129	0.257317467
Po	190	135	134.31	6.95	6.75	0.192520776	0.37037037	0.374185604
At	*	127	122.83	7.6	7.6	*	0.471200942	0.503737971

International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.177
Volume 7 Issue VI, June 2019- Available at www.ijraset.com

Rn	*	120	131.15	8.25	8.25	*	0.572916667	0.47964217
Fr	*	*	444.79	2.2	2.2	*	*	0.011120201
Ra	215	*	343.32	2.85	2.85	0.061654949	*	0.024179463
Ac	195	*	326.15	3	3	0.078895464	*	0.028202427
Th	180	*	310.61	3.15	3.15	0.097222222	*	0.032649737
Pa	180	*	227.56	4.3	4.3	0.132716049	*	0.083037947
U	175	*	197.67	4.95	4.95	0.161632653	*	0.126684556
Np	175	*	174.73	5.6	5.6	0.182857143	*	0.183422696
Pu	175	*	144.96	6.75	5.6	0.220408163	*	0.266496596
Am	175	*	129.15	7.4	7.4	0.241632653	*	0.443652465
Cm	*	*	129.6	7.55	7.55	*	*	0.449507506
Bk	*	*	112.47	8.7	8.51	*	*	0.672753816
Cf	*	*	104.65	9.35	9.35	*	*	0.853754775
Es	*	*	97.85	10	10	*	*	1.0444276
Fm	*	*	91.88	10.65	10.65	*	*	1.261559199
Md	*	*	86.59	11.3	11.3	*	*	1.507103104
No	*	*	81.88	11.95	11.95	*	*	1.782428991
Lr	*	*	80.86	12.1	12.1	*	*	1.850622

It is argued as to which Electronegativity-model is best approximation because no benchmark for this intuitive concept has been set up till date. Furthermore, the confusion as to what physical picture corresponds Electronegativity and even if non-agreement of proposed units such as Energy, Force and Potential. Numerical values of quantities with different units in computation are not comparable because they are conceptually different. No effort is made to compare the computed values of electronegativity with those of other scales. The computed electronegativity values reproduce the periodicity and also increase monotonically right from representative element to noble gas with maximum value.

VI. CONCLUSION

The new attempt to define electronegativity is characterized by specific physical meaning and reliable theoretical basis since it is derived from two famous mathematical formulation i.e Hellmann Feynman theorem and Born Oppenheimer (in turn conventional Hartree Fock) approximation. This definition will be acting like a bridge in between two parallel definitions of electronegativity (either in energy or force). It will be logical to consider electronegativity equalization in a diatomic as well as polyatomic system. This new approach (force approach) will be helpful to assign the more accurate electronegativity values to various elements of the periodic table and also more valuable in different areas of chemical science for example to predict the structure and property of materials. This will also help design new electrode materials efficiently, electrocatalysts with novel properties for energy conversion devices like Fuel cell, Solar cell etc.

VII. ACKNOWLEDGEMENT

A. Nomenclature

E_{hf}	-	Hartree Fork Energy
E_j^A	-	One electron energy of orbital j
f_{AB}	-	Orbital multiplier
f_i	-	Atomic force or overlap force or Screening force
$f_i(R_A)$	-	Atomic force or overlap force or Screening force at R_A
$F(R_A), F(R_B)$	-	Force at position of nuclei A and B
$f(r)$	-	Atomic/overlap/screening force at r, berlin quantity

International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.177
Volume 7 Issue VI, June 2019- Available at www.ijraset.com

F_ς	-	Hellmann-Feynman force
$F_{\varsigma'}$	-	Hellmann-Feynman force (unsteady state)
$F_{\varsigma A}$	-	Hellmann-Feynman on atom A
$F(r)$	-	Sum of electronic kinetic energy and electron repulsion energy functional of density
H_e	-	Electronic Hamiltonian
H^{mol}	-	Molecular Hamiltonian
H_n	-	Nuclear Hamiltonian
s_i	-	Spin coordinate
T	-	Kinetic energy operator
T_e	-	Kinetic energy Operator(electron)
T_n	-	Kinetic energy operator(nucleus)
V_{ee}	-	Electron-electron repulsion term
V_{en}	-	Electron-nuclear attraction term
V_{nn}	-	Nuclear-nuclear repulsion term
x_i	-	Product of space coordinate r_i and spin coordinate s_i of the ith electron

B.   Greek Letters

$\langle\alpha|\zeta|\alpha\rangle$	-	One-electron integral
$\langle\alpha\alpha|\beta\beta\rangle$	-	Two-electron Coulomb integral
$\langle\alpha\beta|\beta\alpha\rangle$	-	Exchange integral
l	-	Parameter of value lying between 0 and 1
$\tilde{N}^2_A$	-	Laplacian operator related to co-ordinate of nucleus A
$\tilde{N}^2_i$	-	Laplacian operator related to Cartesian co-ordinate of electron i
$z(a)$	-	One-electron operator
$h(a,b)$	-	Two-electron operator
ς,ς'	-	Explicit Parameters (steady and Perturbation) in Hamiltonian
V_A	-	Parameter in Hamiltonian for a coordinate of nucleus A
y	-	Wave function
y_n	-	Nuclear wave function
y_e	-	Electronic wave function
$y*$	-	Conjugate wave function
r_0	-	Unperturbed occupancy

REFERENCES

[1] A. L. Allred and E. G. Rochow, "A scale of electronegativity based on electrostatic force," J. Inorg. Nucl. Chem., vol. 5, no. 4, pp. 264–268, Jan. 1958.

[2] L. Pauling, "Atomic Radii and Interatomic Distances in Metals," J. Am. Chem. Soc., vol. 69, no. 3, pp. 542–553, Mar. 1947.

[3] J. C. Slater, "Atomic Shielding Constants," Phys. Rev., vol. 36, no. 1, pp. 57–64, Jul. 1930.

[4] Housecroft C.E. and Sharpe A.G., "Electronegativity values," in Iorganic chemistry, Pearson Education Limited, 2005, p. 38.

[5] R. J. Boyd and G. E. Markus, "Electronegativities of the elements from a nonempirical electrostatic model," J. Chem. Phys., vol. 75, no. 11, pp. 5385–5388, Dec. 1981.

[6] C. Mande, P. Deshmukh, and P. Deshmukh, "A new scale of electronegativity on the basis of calculations of effective nuclear charges from X-ray spectroscopic data," J. Phys. B At. Mol. Phys., vol. 10, no. 12, pp. 2293–2300, Aug. 1977

[7] Y. Zhang, "Electronegativities of Elements in Valence States and Their Applications. 2. A Scale for Strengths of Lewis Acids," Inorg. Chem., vol. 21, no. 11, pp. 3889–3893, Nov. 1982

[8] T. Jecko, "On the mathematical treatment of the Born-Oppenheimer approximation," J. Math. Phys., vol. 55, no. 5, p. 053504, May 2014.

[9] M. Born and R. Oppenheimer, "Zur Quantentheorie der Molekeln," Ann. Phys., vol. 389, no. 20, pp. 457–484, 1927.

[10] E. P. Gyftopoulos and G. N. Hatsopoulos, "Quantum-Thermodynamic Definition of Electronegativity," Proc. Natl. Acad. Sci., vol. 60, no. 3, pp. 786–793, 1968.

[11] M. B. Einhorn and R. Blankenbecler, "Bounds on scattering amplitudes," Ann. Phys. (N. Y)., vol. 67, no. 2, pp. 480–517, Oct. 1971.

[12] M. S. Gopinathan and M. A. Whitehead, "On the Dependence of Total Energy on Occupation Numbers," Isr. J. Chem., vol. 19, no. 1–4, pp. 209–214, 1980.

[13] P. Geerlings, F. De Proft, and W. Langenaeker, "Conceptual Density Functional Theory," Chem. Rev., vol. 103, no. 5, pp. 1793–1874, May 2003.

[14] C. K. Jørgensen, Orbitals in Atoms and Molecules. Academic Press Inc., New York, 1962.

[15] R. T. Sanderson, "An interpretation of bond lengths and a classification of bonds," Science (New York, N.Y.), vol. 114, no. 2973. American Association for the Advancement of Science, pp. 670–672, 1951.

[16] R. Ferreira, "Principle of electronegativity equalization. Part 1.—Bond moments and force constants," Trans. Faraday Soc., vol. 59, no. 0, pp. 1064–1074, Jan. 1963.

[17] N. H. March, "The ground-state energy of atomic and molecular ions and its variation with the number of electrons," in Chemical Hardness, Berlin/Heidelberg: Springer-Verlag, 1993, pp. 71–86.

[18] T. T. Nguyen-Dang, R. F. W. Bader, and H. Essén, "Some properties of the Lagrange multiplier μ in density functional theory," Int. J. Quantum Chem., vol. 22, no. 5, pp. 1049–1058, Nov. 1982.

[19] J. Hinze, "The concept of electronegativity of atoms in molecules," Theor. Comput. Chem., vol. 6,212, Jan.1999.

[20] H. Chermette, "Chemical reactivity indexes in density functional theory," J. Comput. Chem., vol. 20, no. 1, pp. 129–154, Jan. 1999.

[21] P. Hohenberg and W. Kohn, "Inhomogeneous Electron Gas," Phys. Rev., vol. 136, no. 3B, pp. B864–B871, Nov. 1964.

[22] C. F. Kammerer and V. Rousse, "Resolvent Estimates and Matrix-Valued Schrödinger Operator with Eigenvalue Crossings; Application to Strichartz Estimates," Commun. Partial Differ. Equations, vol. 33, no. 1, pp. 19–44, Jan. 2008.

[23] E. B. Wilson, "Four‑Dimensional Electron Density Function," J. Chem. Phys., vol. 36, no. 8, pp. 2232–2233, Apr. 1962.

[24] R. E. Stanton, "Hellmann‑Feynman Theorem and Correlation Energies," J. Chem. Phys., vol. 36, no. 5, pp. 1298–1300, Mar. 1962.

[25] R. P. Feynman, "Forces in Molecules," Phys. Rev., vol. 56, no. 4, pp. 340–343, Aug. 1939. B. M. Deb, "Chapter 1," in The Force concept in chemistry, Van Nostrand Reinhold, 1981, p. Page 9.

[26] D. Andrae, Ed., Hans Hellmann: Einführung in die Quantenchemie. Berlin, Heidelberg: Springer Berlin Heidelberg, 2015

[27] I. N. Levine, Quantum Chemistry, 5th ed. Pearson/Prentice Hall, 2009.

[28] P. Politzer and J. S. Murray, "The Hellmann-Feynman theorem: a perspective," J. Mol. Model., vol. 24, no. 9, p. 266, Sep. 2018.

[29] W. Pauli, "Die allgemeinen Prinzipien der Wellenmechanik," in Quantentheorie, Berlin, Heidelberg: Springer Berlin Heidelberg, 1933, pp. 83–272.

[30] H. Hellmann, "Zur Rolle der kinetischen Elektronenenergie für die zwischenatomaren Kräfte," Zeitschrift für Phys., vol. 85, no. 3–4, pp. 180–190, Mar. 1933.

[31] P. Güttinger, "Das Verhalten von Atomen im magnetischen Drehfeld," Zeitschrift für Phys., vol. 73, no. 3–4, pp. 169–184, Mar. 1932.

[32] E. Schrödinger, "Quantisierung als Eigenwertproblem," Ann. Phys., vol. 385, no. 13, pp. 437–490, Jan. 1926.

[33] A. C. Hurley, "The Electrostatic Calculation of Molecular Energies. I. Methods of Calculating Molecular Energies," Proc. R. Soc. A Math. Phys. Eng. Sci., vol. 226, no. 1165, pp. 170–178, Nov. 1954.

[34] A. C. Hurley, "The Electrostatic Calculation of Molecular Energies. II. Approximate Wave Functions and the Electrostatic Method," Proc. R. Soc. A Math. Phys. Eng. Sci., vol. 226, no. 1165, pp. 179–192, Nov. 1954.

[35] A. C. Hurley, "The Electrostatic Calculation of Molecular Energies. III. The Binding Energies of Saturated Molecules," Proc. R. Soc. A Math. Phys. Eng. Sci., vol. 226, no. 1165, pp. 193–205, Nov. 1954.

[36] A. C. Hurley, "The Electrostatic Calculation of Molecular Energies. IV. Optimum Paired-Electron Orbitals and the Electrostatic Method," Proc. R. Soc. A Math. Phys. Eng. Sci., vol. 235, no. 1201, pp. 224–234, Apr. 1956.

[37] R. F. W. Bader, "Binding Regions in Polyatomic Molecules and Electron Density Distributions," J. Am. Chem. Soc., vol. 86, no. 23, pp. 5070–5075, Dec. 1964.

[38] R. F. W. Bader and W. H. Henneker, "The Ionic Bond," J. Am. Chem. Soc., vol. 87, no. 14, pp. 3063–3068, Jul. 1965.

[39] R. F. W. Bader and H. J. T. Preston, "A CRITIQUE OF PAULI REPULSIONS AND MOLECULAR GEOMETRY," Can. J. Chem., vol. 44, no. 10, pp. 1131–1145, May 1966.

[40] R. F. W. Bader, "THE USE OF THE HELLMANN–FEYNMAN THEOREM TO CALCULATE MOLECULAR ENERGIES," Can. J. Chem., vol. 38, no. 11, pp. 2117–2127, Nov. 1960.

[41] R. F. W. Bader and G. A. Jones, "the Hellmann–Feynman Theorem and Chemical Binding," Can. J. Chem., vol. 39, no. 6, pp. 1253–1265, Jun. 1961.

[42] T. Koga and H. Nakatsuji, "The Hellmann-Feynman theorem applied to long-range forces," Theor. Chim. Acta, vol. 41, no. 2, pp. 119–131, 1976.

[43] T. Koga, H. Nakatsuji, and T. Yonezawa, "Generalized Berlin diagram for polyatomic molecules," J. Am. Chem. Soc., vol. 100, no. 24, pp. 7522–7527, Nov. 1978.

[44] T. Koga, H. Nakatsuji, and T. Yonezawa, "Force and density study of the chemical reaction process $OH_2 + H^+ \rightarrow OH_3^+$," Mol. Phys., vol. 39, no. 1, pp. 239–249, Jan. 1980.

[45] P. Politzer, "A Study of the Bonding in the Hydrogen Molecule [1]," J. Phys. Chem., vol. 70, no. 4, pp. 1174–1178, Apr. 1966.

[46] P. Politzer and K. C. Daiker, "Molecular electrostatic potentials. Negative potentials associated with some methyl and methylene groups," Chem. Phys. Lett., vol. 34, no. 2, pp. 294–297, Jul. 1975

[47] A. J. Coleman, "Structure of Fermion Density Matrices. II. Antisymmetrized Geminal Powers," J. Math. Phys., vol. 6, no. 9, pp. 1425–1431, Sep. 1965.

[48] A. J. Coleman, "INFINITE RANGE CORRELATION AND LARGE EIGENVALUES OF THE 2-MATRIX," Can. J. Phys., vol. 45, no. 3, pp. 1271–1273, Mar. 1967.

[49] A. J. Coleman, "Necessary Conditions for N □Representability of Reduced Density Matrices," J. Math. Phys., vol. 13, no. 2, pp. 214–222, Feb. 1972.

[50] T. Berlin, "Binding Regions in Diatomic Molecules," J. Chem. Phys., vol. 19, no. 2, pp. 208–213, Feb. 1951.

[51] A. Larsen, R. S. Poulsen, and T. P. Garm, "Applied Hartree-Fock methods Atomic and diatomic energy computations," Denmark, 2015.

[52] J. C. Slater, "Atomic Shielding Constants," Phys. Rev., vol. 36, no. 1, pp. 57–64, Jul. 1930.

[53] Koga T,Tatewaki H,Shimazaki T.Chemically reliable uncontracted Gaussian-type basis sets for atoms H to Lr.Chem Phys Lett.2000;328(4-6):473-482.

[54] J. C. Slater, "Atomic Radii in Crystals," J. Chem. Phys., vol. 41, no. 10, pp. 3199–3204, No   [57]   E. Clementi and D. L. Raimondi, "Atomic Screening Constants from SCF Functions," J. Chem. Phys., vol. 38, no. 11, pp. 2686–2689, Jun. 1963. [56] J. C. Slater, "Atomic Radii in Crystals," J. Chem. Phys., vol. 41, no. 10, pp. 3199–3204, Nov. 1964

[55] E. Clementi, D. L. Raimondi, and W. P. Reinhardt, "Atomic Screening Constants from SCF Functions. II. Atoms with 37 to 86 Electrons," J. Chem. Phys., vol. 47, no. 4, pp. 1300–1307, Aug. 1967.

[56] Rahm M, Hoffmann R,Ashcroft NW.Atomic and Ionic Radii of Elements 1-96.Chem-A Eur J.2016;22(41)14625-14632.

[57] D. C. Ghosh, T. Chakraborty, and B. Mandal, "The electronegativity scale of Allred and Rochow: revisited," Theor. Chem. Acc., vol. 124, no. 3–4, pp. 295–301, Oct. 2009.

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Call : 08813907089   (24*7 Support on Whatsapp)