NEW FRONT. CHEM. (2021)
Volume 30, Number 1, pp. 35-46
ISSN 2668-9189; ISSN-L 2393-2171

Former: Ann. West Univ. Timisoara – Series Chem.
ISSN: 1224-9513

Article

STATISTICAL ELECTROCHEMISTRY – A DIFFERENT APPROACH IN DESCRIBING THE STANDARD ELECTRODE POTENTIAL

Marina Alexandra Tudoran
National Institute for Research and Development in Electrochemistry and Condensed Matter, Laboratory of Renewable Energies – Scientific, Str. Prof. Paunescu-Podeanu 144, Timisoara 300569, Romania

ABSTRACT

Due to the growing interest for the multidisciplinary approach in science, it arise the necessity of creating a connection between electrochemistry, computer science and the chemistry of oxidation and reduction. In this context, the present study aims to present a different approach in modeling the standard electrode potential, as a function of atomic radius, Pauling electronegativity and first ionization energy respectively. The obtained results show that electronegativity is a better predictor of standard electrode potential in simple regression, while first ionization energy offers a better prediction when associated with electrical resistivity or thermal conductivity.

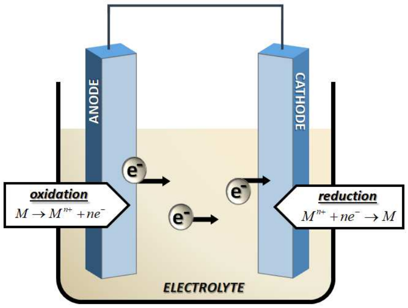
Keywords: electrochemical cell, atomic radius, Pauling electronegativity, first ionization energy, electrode potential.

1. INTRODUCTION

The term "electrochemistry" derives from the terms "electricity" and "chemistry" and is used to describe both a sector of industry and a scientific discipline. In literature, electrochemistry is defined as the science that studies the interactions between chemistry and electricity, i.e. the chemical phenomena coupled with the reciprocal exchanges of electricity. In other words, electrochemistry analyzes and describes the transformations of matter at the atomic scale (i.e. oxidation-reduction reactions), produced as a result of electronic charge changes, controlled by electrical devices [1]. In a different approach, electrochemistry studies the interface processes, which are usually represented by a charge transfer occurring between a solid and a "liquid phase" [2]. Thus, the fundamental process in electrochemistry is considered to be the electrons transfer between the electrode surface and the molecules of a chemical species in the region adjacent to that surface [3].

In general terms, an electrochemical cell (Figure 1) consists in two electrodes immersed in an electrolytic solution. The electrode is represented by the electronic conductor together with its interface with the solution; the anode is considered the electrode that transfers the positive electric charge to the electrolyte, while the cathode is the one that receives the positive electric charge from the electrolyte [4, 5]. The electrolyte consists in the liquid solvent where ions are immersed and is known to strongly affect both the energy of structures and the interface reactions [6].

Figure 1: Schematic representation of an electrochemical cell.



A general definition of an electrochemical reaction states that it is a surface processes triggered by an adequate charge transfer at the liquid/solid interface and involves charged species whose activity depends on the electrostatic potential of the phase species. The reaction generally causes a change in the oxidation state of the participants as a result of an electron transfer; the oxidized species is the one from which an electron is removed, while the reduced species is the one to which the electron is added [7]. Thus, an oxidation-reduction reaction, i.e. redox reaction, involves the transformation of matter resulted from the electrons movement at the atomic level. If a species, or more precisely a chemical element of that species, gains one or more electrons, it is said that it undergoes a reduction process; when the species loses electrons, it is said to undergo an oxidation process. Such transformations are called ***half redox reactions*** and it applies to two species for which a given element exists in two different forms. These two species are called reducer (i.e. Red) and oxidizer (i.e. Ox) and form a redox pair, usually denoted by *Ox/Red*. The global equation of the half redox reaction for the *Ox/Red* couple has the following form: $\mathbf{Red} \rightleftharpoons \mathbf{Ox} + \boldsymbol{n}\mathbf{e}^-$, with Red - the reducer, able to donate electrons, and Ox - the oxidant, able to gain electrons [1].

Electrochemistry is considered a ubiquitous field in everyday life, being present from lithium-ion batteries to biomedical sensors and artificial photosynthesis. However, despite its importance, a complete quantitative and predictive theory has yet to be developed due to the complex physical and chemical phenomena which are present during the electrochemical reactions. Therefore, there is also a difficulty in communicating and quantifying the electrochemical processes occurring at the solid-liquid interface in terms of physics and chemistry. From the physicist's perspective, it is preferable to understand the process by which the physical (band) conduction of a material turns into an event of a chemical electron transfer which occur at the solid-liquid interface, while from the chemist's perspective, one needs to start from the kinetics present in the „liquid" and then evaluate the way in which the charge transfer occurs in a solid. At the same time, considering that over the years a large number of electrochemical cell models obtained through studies focused on specific reactions with specific materials have been used in industry, the aim is to further improve these models so that they can provide higher performance in terms of energy consumption and flow [2, 8].

1.1. Characteristics of electrode materials

The chemical bonding nature and the way in which it determines the physico-chemical properties of the constituted atoms are still in the center of modern chemistry [9]. At the same time, starting from the premise that the association between the properties of atoms or molecules and their geometrical parameters can be made in the conceptual formalism of DFT, the classical macroscopic theories became more and more utilized in explaining the atomic behavior, generally based on the correspondence principle [10].

On the micro level, by measuring the bond lengths, one will obtain the empirical radius called the covalent radius [11], while van der Waals radius is considered to be the distance at which one can measure the interaction between atoms, being correlated with different atomic properties associated with charge distribution. Initially, the atomic radii were defined in order to experimentally reproduce the bonds length. Form the historical perspective, the idea has its roots in the Bohr atomic model, which states that the atomic dimensions are determined by the electron rigid orbits, the Bohr radius being of the form:

$$a_0 = \hbar^2 / m_e e^2 \tag{1}$$

The atomic radii can also be used in modeling ionic conductivity, diffusion, surface tension, preference towards sites, defects and other application dependent of dimension. Despite its limitation, the atomic radius still represents a phenomenological approach with many applications in studies form engineering, physics and chemistry areas [10, 12].

At the same time, it is considered in practice that the atom dimension is associated to the atomic interactions and denotes the distance on which the atomic nuclei can approach each other. Through the repulsive and attraction parts of the potential, this distance is affected, by exchange, scattering or displacement of electrons, all these electronic processes being related to the atoms ability to attract electrons with different strengths, measured through electronegativity [12]. In this context, Pauling made the assumption that the energy of a covalent bond can be divided in ionic and covalent constituents [13]. Thus, he originally defined electronegativity as the power of an atom in a molecule to attract electrons to itself when interacts with other atoms in order to form molecules or solids. At the same time, using the valence bond image of the partial ionic character of covalent bonds, Pauling was able to determine the electronegativity values for a single atom using a thermodynamic approach. In other words, the electronegativity scale obtained by Pauling is based on thermochemical data and is related to the electronic configuration of the selected atoms [14, 15, 16]. Electronegativity is a very important concept in chemistry, physics and other branches of science, due to the fact that it can be used to understand and model many of fundamental properties, such as bond polarity and dipole moment, bond energy, force constant and inductive effects. Recently, this concept has also been used in chemical informatics and materials design [14, 15].

Electron affinity is considered to be another characteristic with major importance in understanding the nature of chemical bonding, defined as the quantity of energy which is released on the addition of an electron to a neutral atom. Another definition of electron affinity states that it represents the difference between the neutral species and the negatively charged ion, i.e. the potential on zero ionization [17], being an important electronic property in different domains of material science, chemistry or physics [18].

At the same time, in literature, the ionization energy (or ionization potential) is defined as the minimum energy which is required to remove an electron from an initial position r to a distance $r \to \infty$, with the specification that the kinetic energy of the respective electron before and after removing is the same [19]. Thus, for a system consisting of N electrons and a nucleus of charge Z, the ionization energy is represented by the formula [20, 21]:

$$I(N,Z) = E(N-1,Z) - E(N,Z) \tag{2}$$

However, unlike other types of energies that can be obtained from calculations, the ionization energy of electrons is the only part of the total energy that can be measured experimentally, its values being available in the literature, being a fundamental property of molecular species, along with the electron affinity [22, 23].

On the macro level, the thermal conductivity (κ) represents a physical parameter which quantifies and characterizes the ability of a material to conduct heat; in case of metals, its general formula is as following:

$$\kappa = \kappa_{ph} + \kappa_e \tag{3}$$

with κ_{ph} – phononic thermal conductivity (associated with lattice vibration) and κ_e – electronic thermal conductivity. In a different approach, thermal conductivity can be directly calculated using Fourier law, if the spatial distance l and the heat reaction flux $\dot{Q}$ are known:

$$\kappa = \frac{\dot{Q}}{A \cdot (\partial T / \partial x)} \tag{4}$$

Thus, elucidating the process of heat conduction on metals and having the possibility of predicting the conduction capacity of a particular alloy are subjects of technological and scientific interest [24, 25].

Another specific property of metals is the electrical resistivity, which can be calculated using the Drude approach. According to the author, is assumed that the electrons are subjected to a viscosity force proportional to their speed, the electrical resistivity on equilibrium ($d\vec{v}/dt = 0$) having the formula:

$$\rho = m / Ne^2\tau \text{, for } \tau = m/\alpha \tag{5}$$

with m – electron mass, e – charge, N – the total electrons number of the compound and τ– the relaxation time [26]. Studies in this area also state that there is an association between the materials general resistivity and the kinetic coefficient σ form the charge transport equation, as following:

$$1/\sigma = \rho = \rho_{e-d} + \rho_{e-ph} + \rho_{e-m} + \ldots \tag{6}$$

with ρ_{e-d} – the contribution due to electrons scattering by defects, ρ_{e-ph} – the contribution due to electrons scattering by phonons, and ρ_{e-m} – contribution due to electrons scattering by magnons [27].

The ***standard electrode potential*** ($E_{O/R}$) of a redox system containing oxidized (O) and reduced (R) species is defined as a measure of the relative oxidation and reduction capacities of those species. Thus, in redox systems with positive potentials, hydrogen is oxidized to protons; in systems with negative potentials, protons are reduced to hydrogen by the reducers (i.e. electron donors) [8]. In physical terms, given an electrode immersed in the electrolyte, the electrode potential represents the energy level of electrons, i.e. Fermi level [28]. Experimentally, there is no direct way to measure the electrode potential, but it can be deduced by measuring the potential difference between a selected electrode and a second electrode with known potential placed in the same solution (cell potential, E_{cell}) [3]. For example, considering the electrode $M^{z+}\middle| M$, the standard electrode potential (E_0) is calculated as the potential difference at 298°K between this electrode and the standard hydrogen electrode, with the following cell reactions [29]:

$$M^{z+}(aq.,\, a=1)+ze=M \tag{7}$$

$$H^{+}(aq.,\, a=1)+e=\tfrac{1}{2}H_2(gas.,\ p=1\ atm) \tag{8}$$

In this case, the standard potential is referring to the potential of a pure metal which is measured using a hydrogen reference electrode [30]. These values also show the voltage for the metal in equilibrium with a solution of its ions having a concentration of 1 mol per liter [31]. The electrode potential is also involved in manipulation of electrochemical reaction rates. The electron transfer rate can be easily changed by several orders of magnitude at a given temperature by a proper control of the electrode potential [32].

2. METHOD

2.1. Theoretical Model

According to its general definition, the correlation coefficient represents a statistical parameter which measures the degree/strength of an association which is assumed to be linear between variables (measured on a unit scale). There are different correlation indices known in literature, but one of the most common is the Person correlation index (r) developed by Karl Pearson starting from the idea initially proposed by Sir Francisc Galton. This index has with values between the interval $[-1,+1]$, a higher absolute value of r indicating that the dispersion points are closer to the regression line, while $r=\pm 1$ is considerate to be the perfect correlation. In practice, the Pearson r^2 coefficient is also used in order to establish how much variance is shared between the considered variables [33, 34, 37].

At the same time, an important objective in the scientific research associated with data analysis imply the possibility to predict values for a random dependent variable based on values of independent variable, through a relationship of statistical nature. The study of this type of functional relationship is called regression [35]. In case of a simple linear regression, values of one variable (dependent/response variable, Y) are estimated based on the values of another variable (independent/predictor variable, X) through a linear equation. The regression model is constructed using the least squares algorithm, i.e. the prediction line describes in which points the sum of square deviation around the function has minimum value and produce the best fitting line associated to X and Y values. The unstandardized linear regression model is as following:

$$Y = a + bX \tag{9}$$

with a – the intercept of the function Y (constant), i.e. the Y value predicted for $X = 0$, b – the slope (regression coefficient), i.e. the X weight for maximize the predictability of Y [34].

An extension of the simple linear regression is represented by the multiple linear regression, obtained by adding two or more predictors in the regression model, as following:

$$Y = a + b_1X_1 + b_2X_2 + \ldots + b_nX_n \tag{10}$$

with a – the regression constant and b_1, b_2, ..., b_n – the partial regression coefficients.

Thus, it can be said that the same fundamental idea can be expressed by both Pearson correlation and linear regression, with the specification that the first one address the degree in which two variable are associated with each other, while the latest is a specific characterization method of a relationship between two variable [33, 34].

2.2. Experimental Model

Among the elements of the periodic table, metals are known to have high electrical conductivity and high reflectivity, these characteristics being explained by the fact that they contain a large number of electrons that can move freely inside the crystal structure build up from the ion-cores with positive charge [36].

Table 1: Physico-chemical parameters of the selected metals

Metal	Atomic radius (Å)	Covalent radius (Å)	χ (Pauling)	Electron affinity (V)	Ist ionization energy (V)
Li	**1.82**	**1.30**	**0.98**	**0.6181**	**5.3918**
Al	**1.84**	**1.24**	**1.61**	**0.4328**	**5.9858**
Fe	**2.04**	**1.24**	**1.83**	**0.1510**	**7.9025**
Ni	**1.97**	**1.17**	**1.91**	**1.1560**	**7.6399**
Cu	**1.96**	**1.22**	**1.90**	**1.2350**	**7.7264**
Ag	**2.11**	**1.36**	**1.93**	**1.3020**	**7.5763**
Sn	**2.17**	**1.40**	**1.96**	**1.1121**	**7.3440**

Starting from this premise, several electrode metals (whit their associated half reaction) were chosen for the present study, each being characterized by different physico-chemical parameters starting from micro to macro level: atomic and covalent radius, Pauling electronegativity, electron affinity, first ionization energy, electrical resistivity, thermal conductivity and standard electrode potential (Table 1 and Table 2). All values were available in literature [38, 39, 40, 41].

In order to establish the relationship between the electrode potential and the other properties of metals, first we determine the degree of their correlation, by calculating the Pearson correlation coefficient (Table 3). One sample Kolmogorov-Smirnov test (Figure 2) was applied prior to the correlation analysis, to verify if the selected parameters are normally distributed.

Table 2: Electrochemical parameters of the selected metals

Metal	**Half reaction (at 25°C)**	**Electrical resistivity ($\times 10^{-8}$ Ωm)**	**Thermal conductivity ($Wm^{-1}K^{-1}$)**	**Standard electrode potential (V)**
Li	$\mathbf{Li}^{+}(aq) + \mathbf{e}^{-} \rightleftharpoons \mathbf{Li}(s)$	9.5	85	- 3.040
Al	$\mathbf{Al}^{3+}(aq) + \mathbf{3e}^{-} \rightleftharpoons \mathbf{Al}(s)$	2.7	235	-1.676
Fe	$\mathbf{Fe}^{2+}(aq) + \mathbf{2e}^{-} \rightleftharpoons \mathbf{Fe}(s)$	10	80	-0.44
Ni	$\mathbf{Ni}^{2+}(aq) + \mathbf{2e}^{-} \rightleftharpoons \mathbf{Ni}(s)$	7.2	91	-0.257
Cu	$\mathbf{Cu}^{2+}(aq) + \mathbf{2e}^{-} \rightleftharpoons \mathbf{Cu}(s)$	1.72	400	0.3419
Ag	$\mathbf{Ag}^{+}(aq) + \mathbf{e}^{-} \rightleftharpoons \mathbf{Ag}(s)$	1.63	430	0.7996
Sn	$\mathbf{Sn}^{2+}(aq) + \mathbf{2e}^{-} \rightleftharpoons \mathbf{Sn}(s)$	11.5	66.6	66.6

The multiple regression was used in order to determine how much variation in standard electrode potential can be explained by variability in the initial independent variables along with electrical resistivity and thermal conductivity. Thus, all the regression equations were constructed by multiplying the individual slopes with the values of the independent variables and then add the obtained products to the intercept. All calculations were made using IMB SPSS program.

3. RESULTS AND DISCUSSIONS

The values obtained for the significance level of the one sample Kolmogorov-Smirnov test indicate that all variables in the study are normally distributed, thus we could apply the Pearson statistic in order to investigate if there is a statistically significant association between the independent and dependent variables. From the results obtained for the Pearson coefficient, one can state that in all cases, the direction of the correlation is positive, and the effect size is moderate and large for almost all parameters.

Table 3: Pearson correlation coefficients

	Atomic radius	***Covalent radius***	***χ (Pauling)***	***Electron affinity***	***1st ionization energy***
Standard electrode potential	0.780	0.093	0.935	0.597	0.914

Based on the effect size, we further consider as the independent variable the parameters with higher correlation coefficient; worth mentioning, due to the fact that electron affinity and electronegativity are both related to the same fundamental idea, we selected only the Pauling electronegativity as a predictor of the standard electrode potential. Thus, ***simple linear regression*** was conducted in order to investigate how well atomic radius predicts standard electrode potential. The identified equation to understand this relationship is of the form:

$$E^{\ominus}_{r_{at}} = -16.209 + 7.840 \times r_{at}, \; R = 0.780, \; R^2 = 0.608 \tag{11}$$

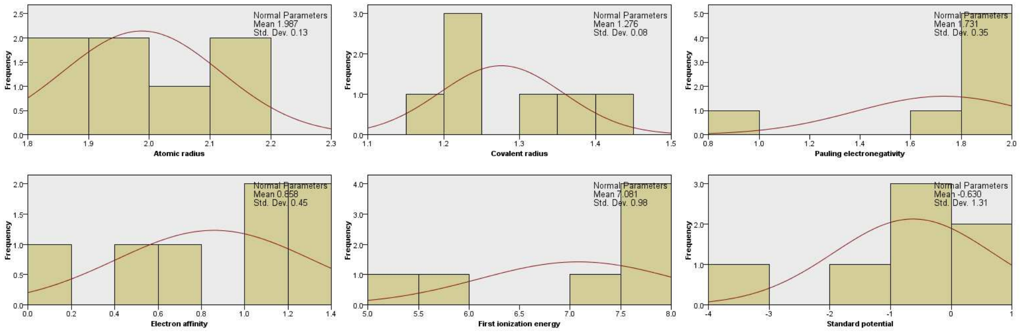
The R value corresponds to the Pearson correlation coefficient, and R^2 value indicates that 60.8% of the variance in standard electrode potential is attributed to atomic radius.

Same method was applied for investigate the relationship between Pauling electronegativity and standard electrode potential, the regression equation being:

$$\mathrm{E}^{\Theta}_{\chi_P} = -6.665 + 3.485 \times \chi_P,\ R = 0.935,\ R^2 = 0.874 \tag{12}$$

with R indicating a strong correlation between these two variables, and R^2 indicating that 87.4% of the variance in standard electrode potential is attributed to Pauling electronegativity.

Figure 2: One sample Kolmogorov-Smirnov test.



Also, we consider first ionization energy as independent variable in order to predict the standard electrode potential, with the following regression equation:

$$\mathrm{E}^{\Theta}_{E_I} = -9.275 + 1.221 \times E_I,\ R = 0.914,\ R^2 = 0.835 \tag{13}$$

in this case, the Pearson coefficient is smaller compared to the one obtained for the electronegativity model but higher than the one from atomic radius model, and only 83.5% of the variance in standard electrode potential can be attributed to the ionization energy.

Based on the results obtained in case of simple linear regression, it was determined that Pauling electronegativity is a better predictor for standard electrode potential. In order to test the validity of this model, the predicted values were computed and the regression line was constructed and compared with the one obtained for the observed values (Figure 3a).

We wanted to see if whether or not the models obtained can be further improved by adding other parameters in the simple linear regression equations, i.e. electrical resistivity and thermal conductivity. Thus, ***multiple linear regression*** was applied in order to predict the standard electrode potential values based on atomic radius and electrical resistivity (14), and thermal conductivity respectively (15). The identified equations are of the form:

$$\mathrm{E}^{\Theta}_{r_{at}} = -17.328 + 8.921 \times r_{at} + (-0.163) \times \rho,\ R = 0.935,\ R^2 = 0.873 \tag{14}$$

$$\mathrm{E}^{\Theta}_{r_{at}} = -16.367 + 7.541 \times r_{at} + 0.004 \times \kappa,\ R = 0.905,\ R^2 = 0.819 \tag{15}$$

In his case, the R value represents the correlation coefficient when both independent variables ("atomic radius" and "electrical resistivity"/thermal conductivity) are taken together and compared with the dependent variable "standard electrode potential", being higher in both cases compared to the value obtained for simple linear regression. R^2 value indicates that 87.3% (81.9% respectively) of the variance in standard electrode potential is explained by the new model.

In the same way the multiple regression was computed for Pauling electronegativity along with electrical resistivity (16) and thermal conductivity (17), and the following equations were obtained:

$$\mathrm{E}^{\Theta}_{\chi_P} = -6.167 + 3.365 \times \chi_P + (-0.046) \times \rho\,,\ R = 0.946,\ R^2 = 0.894 \tag{16}$$

$$\mathrm{E}^{\Theta}_{\chi_P} = -6.592 + 3.205 \times \chi_P + 0.002 \times \kappa\,,\ R = 0.965,\ R^2 = 0.932 \tag{17}$$

One can notice that *R* and *R*² values in both regression models are higher compared to the case of simple regression, being also higher than the values obtained in case of the multiple regression model with the atomic radius.

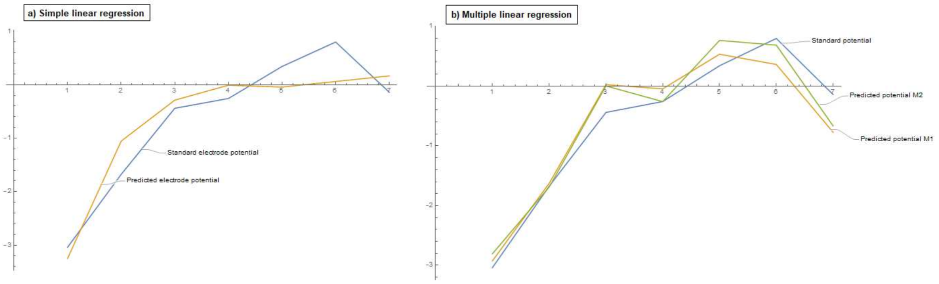
Also, the influence of electrical resistivity (18) and thermal conductivity (19) in predicting the standard electrode potential along with first ionization energy were analyzed and the following models were obtained:

$$\mathrm{E}^{\Theta}_{E_I} = -8.533 + 1.193 \times E_I + (-0.087) \times \rho\,,\ R = 0.955,\ R^2 = 0.912 \tag{18}$$

$$\mathrm{E}^{\Theta}_{E_I} = -9.134 + 1.126 \times E_I + (-0.003) \times \rho\,,\ R = 0.967,\ R^2 = 0.935 \tag{19}$$

The *R* value in both cases shows a *strong* multiple correlation coefficients, the variance in standard electrode potential being the highest among the three models.

Figure 3: a) Electrode potential as a function of Pauling electronegativity; b) Electrode potential as a function of first ionization energy and electrical resistivity (M1) and thermal conductivity (M2), respectively.



Following the same principle used in case of simple regression, the best fit model, in this case the one containing the first ionization energy, was used to compute de predicted values for electrode potential and the regression line, which was also compared with the regression line for the observed values (Figure 3b). The results show that when considered a single variable, the best association was observed between the electrode potential and the Pauling electronegativity. On the other hand, in case of multiple linear regression, the ionization energy appears to be a better predictor when combined with electrical resistivity and thermal conductivity. Also, the values for *R* and R^2 were close in case when thermal conductivity was added in the regression model for ionization energy and Pauling electronegativity.

4. CONCLUSION

The aim of this study is to give a different perspective on the way in which the standard electrode potential can be computationally predicted using the phisyco-chemical properties available in literature as descriptors. The regression model was constructed with one and two independent variables. The results obtained for R and R^2 in case of simple linear regression were smaller compared with the ones obtained for multiple linear regression, proving that adding more independent variables improves the predictive power of the regression.

In conclusion, it can be stated that the standard electrode potential of the studied metals is highly dependent on electronegativity, on one hand, and on first ionization energy along with electrical resistivity and thermal conductivity respectively, on the other hand; the results obtained for the predicted values are very close to the ones for the observed values. Also, the proposed models are in accordance with the electrochemical processes occurring on the electrode surface when in contact with the electrolyte.

ACKNOWLEDGEMENT(S)

MAT addresses hearty thanks to Prof. Dr. Dr. Habil. PI-1 Mihai V. PUTZ from West University of Timişoara and R&D National Institute for Electrochemistry and Condensed Matter - Timişoara for the useful insight and enriching discussions on the electrochemistry domain.

REFERENCES

1. Lefrou, C.; Fabry, P.: Poignet, J.C. *Electrochemistry. The Basics, with Examples*. Springer-Verlag Berlin Heidelberg, 2012, ch. 1, pp. 1-8.
2. Bevan, K.H.; Hossain, S.; Iqbal, A.; Wang, Z. Exploring Bridges between Quantum Transport and Electrochemistry. I. *Journal of Physical Chemistry C* **2016**, *120*, 179-187.
3. Pollet, B.G.; Curnick, O.J. Introduction to Electrochemistry. In *Power Ultrasound in Electrochemistry: From Versatile Laboratory Tool to Engineering Solution, First Edition*. Pollet B.G. Ed.; John Wiley & Sons Ltd, 2012, pp. 1-20.
4. Sato N. Electrochemical Cells. In *Electrochemistry at Metal and Semiconductor Electrodes*; Elsevier Science, 1998, ch. 6, pp. 201-211.
5. Cheng, J.; Sprik, M. Alignment of electronic energy levels at electrochemical interfaces. *Physical Chemistry Chemical Physics* **2012**, *14*, 11245-11267.
6. Sundararaman, R.; Goddard, W.A.; Arias, T.A. Grand canonical electronic density functional theory: algorithms and applications to electrochemistry. *Journal of Chemical Physics* **2017**, *146*, 114104(1-14).
7. Kee, R.J.; Coltrin, M.E.; Glarborg, P.; Zhu, H. Electrochemistry. In *Chemically Reacting Flow: Theory, Modeling, and Simulation, Second Edition*; John Wiley & Sons, Inc., 2018, ch. 18, pp. 613-650.
8. Scott, K. Electrochemistry and Sustainability. In *Handbook of Green Chemistry and Technology*. Clark J., Macquarrie D. Eds.; Blackwell Science Ltd, 2002, ch. 19, pp. 433-465.

9. Joy, J.; Danovich, D.; Kaupp, M.; Shaik, S. Covalent vs charge-shift nature of the metal−metal bond in transition metal complexes: a unified understanding. *Journal of the American Chemical Society* **2020**, 1*42*, 12277−12287.
10. Szarek, P.; Grochala, W. Most probable distance between the nucleus and HOMO electron: the latent meaning of atomic radius from the product of chemical hardness and polarizability. *Journal of Physical Chemistry A*, **2014**, *118*, 10281−10287.
11. DeKock, R.L.; Strikwerda, J.R.; Yu, E.X. Atomic size, ionization energy, polarizability, asymptotic behavior, and the Slater–Zener model. *Chemical Physics Letters* **2012**, *547*, 120–126
12. Szarek, P.; Witkowski, M.; Wozniak, A.P. Unconventional look at the diameters of quantum systems: could the characteristic atomic radius be interpreted as a reactivity measure? *Journal of Physical Chemistry*. C, **2019**, *123*, 11572−11580.
13. Zueva, E.M.; Galkin, V.I.; Cherkasov, A.R.; Cherkasov, R.A. Physical interpretation of the electronegativity. *Russian Journal of Organic Chemistry*, **2002**, *38*, 613-623.
14. Qteish, A. Electronegativity scales and electronegativity-bond ionicity relations: A comparative study. *Journal of Physical Chemistry Solids* **2019**, *124*, 186-191.
15. Sacher, E.; Currie, J.F. A comparison of electronegativity series. Journal of *Electron Spectroscopy and Related Phenomena* **1988**, *46*, 173-177.
16. Ohwada, K. On the Pauling electronegatmty scales-II**.** *Polyhedron* **1984**, *3*, 853-859.
17. Batsanov, S.S.; Batsanov, A.S. *Introduction to Structural Chemistry*. Springer, 2012, ch. 1, pp. 1-12.
18. Hajgató, B.; Deleuze, M.S.; Tozer, D.J.; De Proft, F. A benchmark theoretical study of the electron affinities of benzene and linear acenes. *Journal of Chemical Physics*, **2008**, *129*, 084308;
19. Arulsamy, A.D. Physical properties of titanates, semiconductors and nickelates derived from ionization energy theory. *Physics Letters A*, **2020**, *384*, 126917
20. Gooch J.W. *Encyclopedic Dictionary of Polymers, 2nd ed.* Springer-Verlag New York, 2011, pp. 396.
21. Seco, L.A.; Sigal, I.M.; Solovej, J.P. Bound on the Ionization Energy of Large Atoms. *Communications in Mathematical Physics* **1990**, *131*, 307-315.
22. Zadeh, D.H. Atomic shells according to ionization energies. *Journal of Molecular Modeling* **2019**, *25*, 251(1-7).
23. Tschurl, M.; Boesl, U.; Gilb, S. The electron affinity of phenanthrene. *Journal of Chemical Physics*, **2006**, *125*, 194310.
24. Yang, J. (2004) Theory of Thermal Conductivity. In *Thermal Conductivity - Theory, Properties, and Applications*. Tritt, T.M. ed.; Kluwer Academic /Plenum Publishers, New York, ch. 1, pp.1-22.
25. Belova, I.V.; Veyhl, C.; Fiedler, T.; Murch, G.E. Analysis of anisotropic behaviour of thermal conductivity in cellular metals. *Scripta Materialia*, **2011**, *65*, 436–439.
26. Kenkre, V.M.; Dresden, M. Theory of electrical resistivity. *Physical Review A*, **1972**, *6*, 769-775.
27. Palchaev, D.K.; Murlieva, Zh.Kh.; Kazbekov, K.K. The correlation between electrical resistivity of metals and thermal deformation. *High Temperature*, **2007**, *45*, 632–638.

28. Sato, N. Basics of Corrosion Chemistry. In *Green Corrosion Chemistry and Engineering: Opportunities and Challenges, First Edition.* Sharma S.K., Ed.; Wiley-VCH Verlag GmbH & Co., 2012, ch. 1, pp. 1-32.
29. Burrows, H.D. On the relationship between standard electrode and ionization potentials of metal ions. *Journal of Chemical Education* **1976**, *53*(6), 365.
30. Ahmad, Z. Basic Concepts in Corrosion. In *Principles of Corrosion Engineering and Corrosion Control*; Elsevier Ltd, 2006, ch. 2, pp. 9-56.
31. Jones, D.R.H.; Ashby, M.F. Wet Corrosion of Materials. In *Engineering Materials 1 - An Introduction to Properties, Applications and Design*, 5th edition; Elsevier Ltd., 2019, ch. 27, pp. 431- 447.
32. Atobe, M. Fundamental Principles of Organic Electrochemistry: Fundamental Aspects of Electrochemistry Dealing with Organic Molecules. In *Fundamentals and Applications of Organic Electrochemistry: Synthesis, Materials, Devices, First Edition*. Fuchigami T., Atobe M., Inagi S. Eds.; John Wiley & Sons, Ltd, 2015, ch. 1, pp. 1-10.
33. Kinnear, P.R.; Gray, C.D. *Spss 12 Made Simple*. Psychology Press, 2004, ch. 11, 12, pp. 314, 341-353.
34. Meyers, L.S.; Gamst, G.C.; Guarino, A.J. *Performing Data Analysis Using IBM SPSS*. John Wiley & Sons, Inc., 2013, ch. 22, 24, 26, pp. 159, 173-174, 191.
35. Marques de Sá, J.P. *Applied Statistics Using SPSS, STATISTICA, MATLAB and R*. Springer, 2007, ch. 7, pp. 271-289.
36. Kiejna, A.; Wojciechowski, K.F. *Metal Surface Electron Physics*; Elsevier Science Ltd, 1996, ch. 4, pp. 53.
37. Dudaş, N.A.; Ori, O.; Putz, M.V. Topo-chemical reactivity study on molecular machines. *New Frontiers In Chemistry*, **2020**, *29*(2), 69-97.
38. https://en.wikipedia.org/wiki/Electronegativities_of_the_elements_(data_page)#Electronegativity_(Pauling_scale)
39. https://www.webelements.com/index.html
40. https://www.rsc.org/periodic-table/
41. http://hyperphysics.gsu.edu/hbase/Tables/electpot.html