Pseudo-classification of natural elements and atomic total energy prediction

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Research Article

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Abstract

Technological progression requires looking for new matters that meet specific properties. Moreover, the forecasting of physical and chemical compounds formation and proprieties can base on Datamining methods. In this paper, we use one of the unsupervised methods of Datamining, like Principal Component Analysis (PCA). The first goal is to make pseudo-classification of natural and synthetic elements of periodic table based on their all physicochemical and energies available properties. Likewise, the second goal is to test the effectiveness of this statistical method to estimate correlations and to appreciate the relationships between the properties. A pseudo-classification of periodic elements is a new way of seeing Mendeleev's table. At the end of this work, we present a predictable polynomial that allows the scientific community to make atomic total energy predictions for each natural periodic element, from Z=2 to Z=103.

1. Introduction

The discovery of chemical elements and their classification philosophy had started for decades or more. Thirty-three of elements and substances were reported by Lavoisier in (1743–1794) where he described elements treatment in chemical [1].

In 1807–1808, Davy isolated sodium, potassium, barium, strontium, and calcium through electrolysis [2.].

Like Davy's research, Döbereiner defined traid law to notice the correlation between bromine, iodine, chlorine, sulfur, tellurium, selenium [3.].

It was just waiting for John Dalton; to know that the chemical elements are described by their atomic weights [4]. However, Gay-Lussac in 1809 [5] and Avogadro in 1911 [6] introduced notions on physicochemical properties and differentiation of molecules or atoms. The symbolic representation of the elements was proposed by Berzélius in 1814 [7].

The notion of an atomic mass system and the molecule were in 1860 in the first international congress of chemistry in Karlsruhe [8]. In 1867, the Russian chemist Dmitry Mendeleev selected a professor of mineral chemistry at the University of St. Petersburg after achieving his work on the density of gases and the spectroscope of Gustav Kirchhoff [9–12]. He vertically classified the natural elements already determined in his time according to atomic number and atomic mass.

Thus, he predicted the properties of some missing natural elements from those of their neighbours or traid law.

A review on forms illustrations of the periodic elements during 100 years, is reported by Mazurs 1974 [13].

The Graphic illustration as Spiral and Blocks of the periodic elements are described by Imyanitov 2016 [14]. The philosophy and possibility of improvement of the periodic table are reported recently by Scerri 2020 [15].

The periodicity of natural elements and the introduction of quantum mechanics are fundamental concepts of chemical elements reported by authors (Scerri 2020 15; Pyykkö 201917; Imyanitov 2016 14; Mazurs 1974 13; van Spronsen 1969 16) [13–17].

The periodic table of the elements or the Mendeleev table, which corresponds to the arrangement of chemical elements, is defined to respect a periodicity specific. Currently, in 2020, the periodic table has 118 chemical elements, which is not a fixed limit that is updated each time.

The classical arrangement of natural elements defines that the chemical element with the same number of valence band electrons assemble in the same columns.

The horizontal classification is established based on increasing numbers of electrons from top to bottom then left to right.

Mendeleev's table is probably the earliest example of used data analysis technique in materials science.

In this work, we use the unsupervised classification of periodic elements of Mendeleev's table by using the principal component analysis (PCA) method.

Our goal is to analyze correlations between the physical properties of elements.

In the same way, we try to see if the classification of the elements can be other vision than Mendeleev's classification. At the end of this paper, we extract the correlations between the atomic energies to estimate the Total Energy, only in function of atomic number that can enhance electronic structure calculations methods of elements, especially in condensed Matter Physics discipline.

2. Classification Method

In this work, we use one of the methods of Datamining, Principal Component Analysis PCA [18–22].

3. Results And Interpretation

Figure 1 and Figure 2 present the diagram of properties (Scores plot) and diagram of elements (loading plot), respectively that based on experimental data [23].

It allows us to detect the correlations between the 22 physical properties of the elements, which we noted Var1 to Var22 for better visibility of the diagram. The list of variables is as follows:

We can notice some correlations and anti-correlations. Some of these correlations are simple to explain. Others reflect intrinsic physical principles and relationships. In the list of correlations, we find:

-Var1 correlated to Var2: The atomic number and the atomic mass are correlated.

It's completely normal, as long as the atomic mass includes the sum of the masses of neutrons and protons. The number of these latter is precisely the atomic number Z.

-Var 1 and Var2 correlated to Var 16:

The heat capacity, atomic number, and atomic mass are correlated, which can explain as follows: The heat capacity expresses the ability of the material to assimilate heat.

The principal mode of heat energy assimilation is the phonons or vibrations of the network. The heavy atoms need more energy for exciting the phonons. In other words, they need more heat absorbed for giving a temperature increase.

-Var21 and Var 19 are correlated:

The melting temperature and the boiling temperature have a physical relationship. It is axiomatical, as long as the boiling occurs after fusion.

-Var19 and Var 21 have a relationship with Var20:

The melting and boiling temperatures correlate to the change in enthalpy at melting.

This last quantity expresses the energy which supplies so that the material passes from the solid to the liquid state.

Var13 and Var14 correlated to Var 9:

The elastic constants C11 and C12 and Young's modulus have relationships.

The two constants define the material response to deformation on the atomic scale. Young's modulus is the macroscopic response of the material to tensile deformation. Unquestionably, the macroscopic mechanical behaviour properties are expressions of the displacement of atoms on a smaller scale when applying an external constraint.

-Var4 correlated to Var5: electronegativity and the energy of the 1st ionization are correlated. An electronegative material tends to attract electrons from other atoms in a bond. A fortiori, the electrons of its last layer are strongly linked and are only very difficult to yield that expressed by high ionization energy.

-Var6 correlated to Var8: The network parameter and the molar volume are correlated, which is logic since the interatomic spacing is function volume.

-Var17, Var6, and Var8 are correlated:

The entropy has a relationship with the network parameter. Therefore, with the molar volume. It's' implies that the increase in molar volume increases the disorder in the system.

-Var10 correlated to Var11 and Var12: the elasticity constants S11, S12, and S44 are all correlated. This fact is consistent as long as all these quantities are directly related to how the structure varies when the external stress is applied. In other words, they all arise from the interatomic bond.

On the other hand, we find the anti-correlations

-Var14 has an inverse correlation to Var6 and Var8:

Young's module has an inverse correlation to the network parameter and the molar volume.

It's known from experience that Young's module is proportional to the compression module that measures the network compressibility. So as important as it is, it is difficult to compress the network.

When the lattice parameter and the molar volume decrease, the volume per atom also decreases. By consequence, the atom's possibility to bring closer together decreases.

It explains why the network parameter decreases the compression module as much, and therefore Young's module increases.

-Var1 and Var2 have an inverse correlation with Var4 and Var5: the atomic number and mass are inversely proportional to the electronegativity and the energy of first ionization.

When the number of electrons in the atom increases, the distance between the valence electrons and the nucleus increases.

Consequently, the decreases of electrons implied less energy required to tear them away (first ionization energy) decreases.

Also, when the number of electrons increases, the electronegative decreases, and its' nucleus doesn't attract electrons from neighbouring atoms more strongly.

4. Three-dimensional Representation Of The Variable Diagram

Following Fig. 2, we note that the distribution of the elements in the graph does not follow a particular logic.

The large number of properties used in our analysis is likely responsible for the variability of these results.

Hence, it is very likely that the large number of properties used in our analysis is responsible for the variance of the results and the classification of the items, although original, is not very evident.

Following this introspection, we decided to redo an analysis on all the elements of the periodic table by including this time in a database a more restricted set of properties and which are basic intrinsic properties. More particularly, this time, we have included: the total energy of the atom, the kinetic energy of the electrons, the coulomb energy, and the energy of exchange and correlation of the electronic system.

5. Correlation Of The Atomic Energy And Electronic System

We have collected in a database based on LDA calculations [24]: the total energy, coulombian, kinetic, exchange, and correlation energy for 92 elements ranging from Hydrogen to Uranium. Figure 3 represents the properties plot (score plot). We can see that the atomics energies are distributed practically only along the axis PC1.

We can see that the energies are distributed practically only along the axis PC1. The electron nucleus electrostatic interaction energy and the total energy are on the positive side of PC1, while the kinetic energy and the electron electrostatic interaction energy are on the negative side of PC1.

The energy of exchange and correlation is also on the right side, but with a few components according to PC2. The matrix shown in Figure 4 illustrates correlation types between energies.

Figure 5 represents the diagram of variables (loadings plot).

We have to zoom in on a few areas for good visualization of the points cloud of arrangement of the elements.

As *it's shown in* figure 5, the elements of the periodic table are aligned according to their atomic number, starting from hydrogen and up to uranium in the opposite direction of the PC1 axis.

Also, according to PC2, they form a kind of bell towards the positive direction of PC2. We can explain this as follows: the negative direction of the PC1 axis is correlated with the electron-electron interaction energy and kinetic energy of the electrons, so the elements with more electrons move in this direction.

The distribution curvature of the elements shows too the heaviest elements.

The energy of Coulomb interaction counts more than the energy of exchange and correlation because there are too many electrons.

It is also the case for the lightest elements, where there aren't enough electrons to energy exchange and correlation.

For the middle of elements, the exchange and correlation energy matter more than the coulomb energy, so the positions of elements are shifted upwards.

$$E\ total\text{-}\mathrm{Predict} = (p1*z^{10} + p2*z^{9} + p3*z^{8} + p4*z^{7} + p5*z^{6} + p6*z^{5} + p7*z^{4} + p8*z^{3} + p9*z^{2} + p10*z + p11)*10^{5} \quad (1)$$

Table I shows Atomic total energy predicts using polynomial equation (1) shown in figure 6. Following the error arrange, the results match NIST Standard Reference Database from Z=2 to Z=103 [23-24].

Table I

z	*Coefficients p*	*Etot predicts Hartree*	*Etot Hartree "LDA"*[13-24].	*SD*
93	*3.67E-20*	*-26374.2130385254*	*-26325.4386967855*	*0.18%*
94	*-2.00E-17*	*-27054.7117761243*	*-27002.6683849033*	*0.19%*
95	*4.51E-15*	*-27745.9078872578*	*-27689.6834855652*	*0.20%*
96	*-5.51E-13*	*-28448.1151881729*	*-28386.4092359141*	*0.22%*
97	*3.99E-11*	*-29161.6974796868*	*-29093.9325964725*	*0.23%*
98	*-1.76E-09*	*-29887.0721625673*	*-29811.2722013778*	*0.25%*
99	*4.91E-08*	*-30624.7135474639*	*-30538.8250815148*	*0.28%*
100	*-1.07E-06*	*-31375.1557599997*	*-31276.6433895199*	*0.31%*
101	*-6.11E-06*	*-32138.9951310089*	*-32024.7791035710*	*0.36%*
102	*5.46E-06*	*-32916.8919507090*	*-32783.2840569287*	*0.41%*
103	*-6.44E-06*	*-33709.5714538646*	*-33551.5868267897*	*0.47%*

6. Conclusions

- We have presented the use of a data mining method known as Principal Component Analysis (PCA).
- We have built up a database based on the physical properties of the periodic elements table.
- PCA method using gives us the chance to analyze the database and visualize results on graphs to examine relationships between item properties.
- We have proposed a new pseudo-classification of natural and synthetic elements.
- We applied PCA on a database of the total, kinetic, electrostatic, and exchange energy and correlation of periodic elements until z = 92.
- The kinetic energy and electron-electron interaction energy characterize the heavy elements.
- The electron nucleus interaction energy and the total energy characterize the light elements.
- The energy of exchange and correlation has a particular impact on the distribution of the elements on the loading plot.
- The predicted polynomial allows predicting the total energy for each element of the periodic table only in function of atomic number from Z = 2 to Z = 103.

Declarations

Acknowledgment

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Nomenclature

Var1: Atomic number Z

Var2: Atomic mass

Var3: The states of oxidation

Var4: Electronegativity

Var5: The 1st ionization energy

Var6: The network parameter

Var7: The number of atoms per cell

Var8: The molar volume

Var9: Young's module

Var10: The observation of elasticity S11

Var11: The finding of elasticity S44

Var12: The observation of elasticity S12

Var13: The elasticity module C11

Var14: The elasticity module C44

Var15: Thermal conductivity

Var16: Molar capacity Cp

Var17: Standard entropy S0

Var18: The Enthalpy difference H298-H0

Var19: The melting temperature

Var20: The change in enthalpy at fusion

Var21: The boiling temperature

Var22: The change in enthalpy at boiling point

The authors declare no competing interests.

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Figures

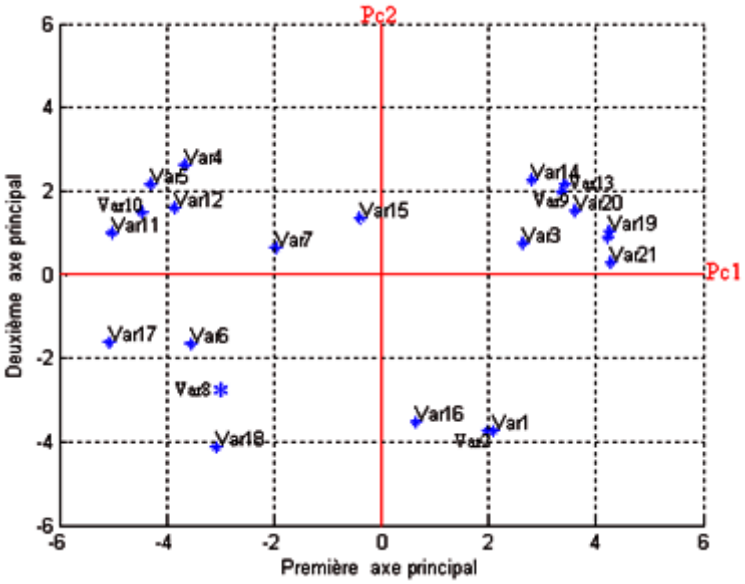

Figure 1

The correlation between physical properties – Scores plot

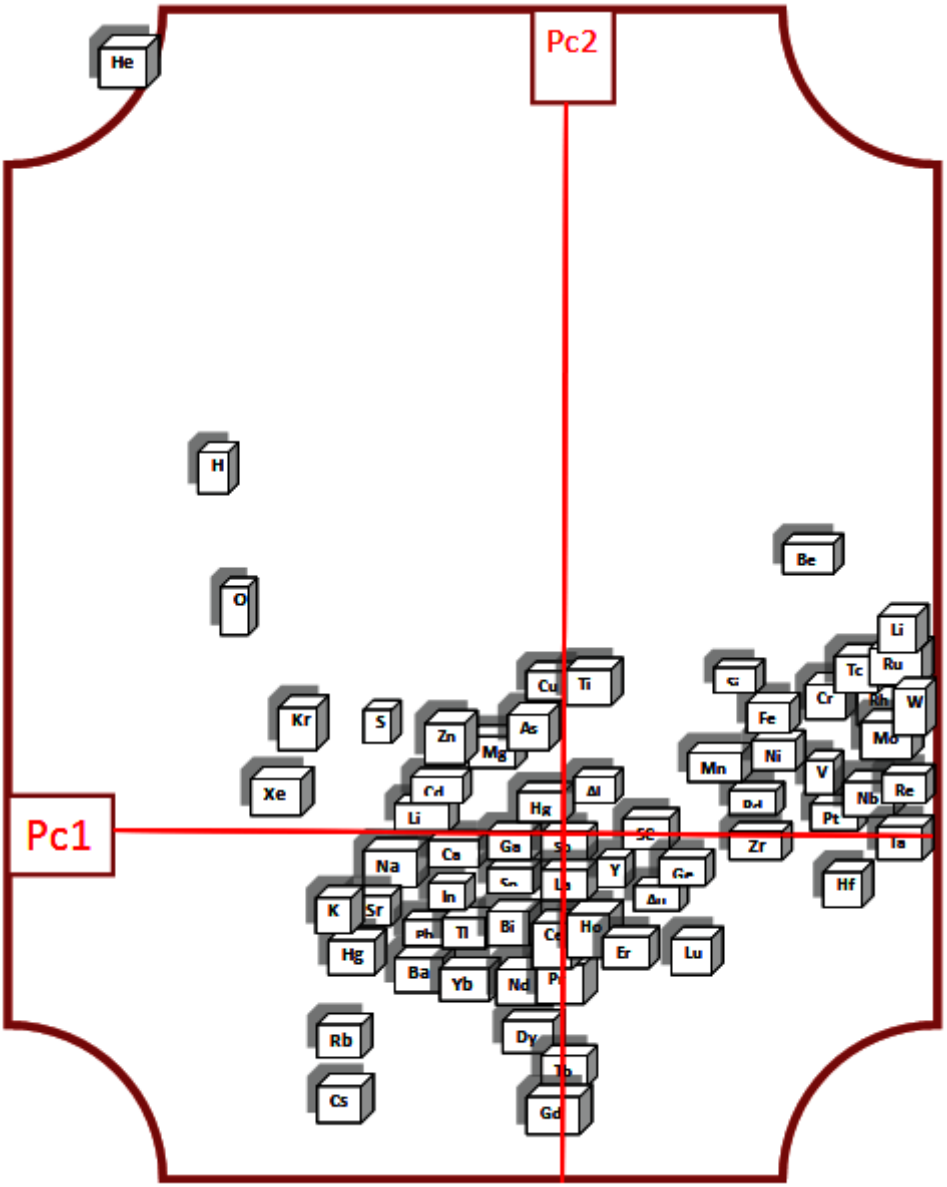

Figure 2

Three-dimensional variable (loading plot)

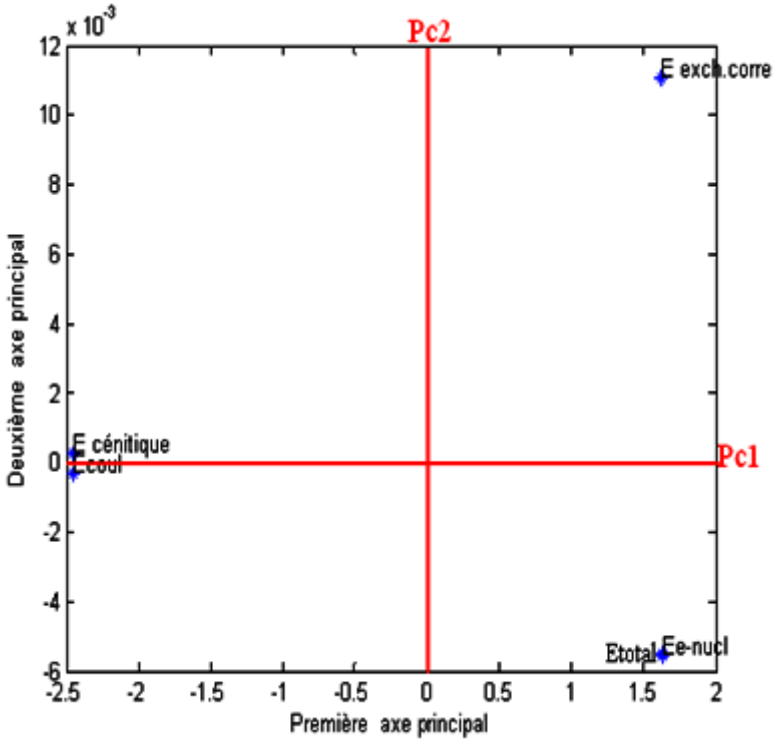

Figure 3

Correlation between electronic properties - Scores plot

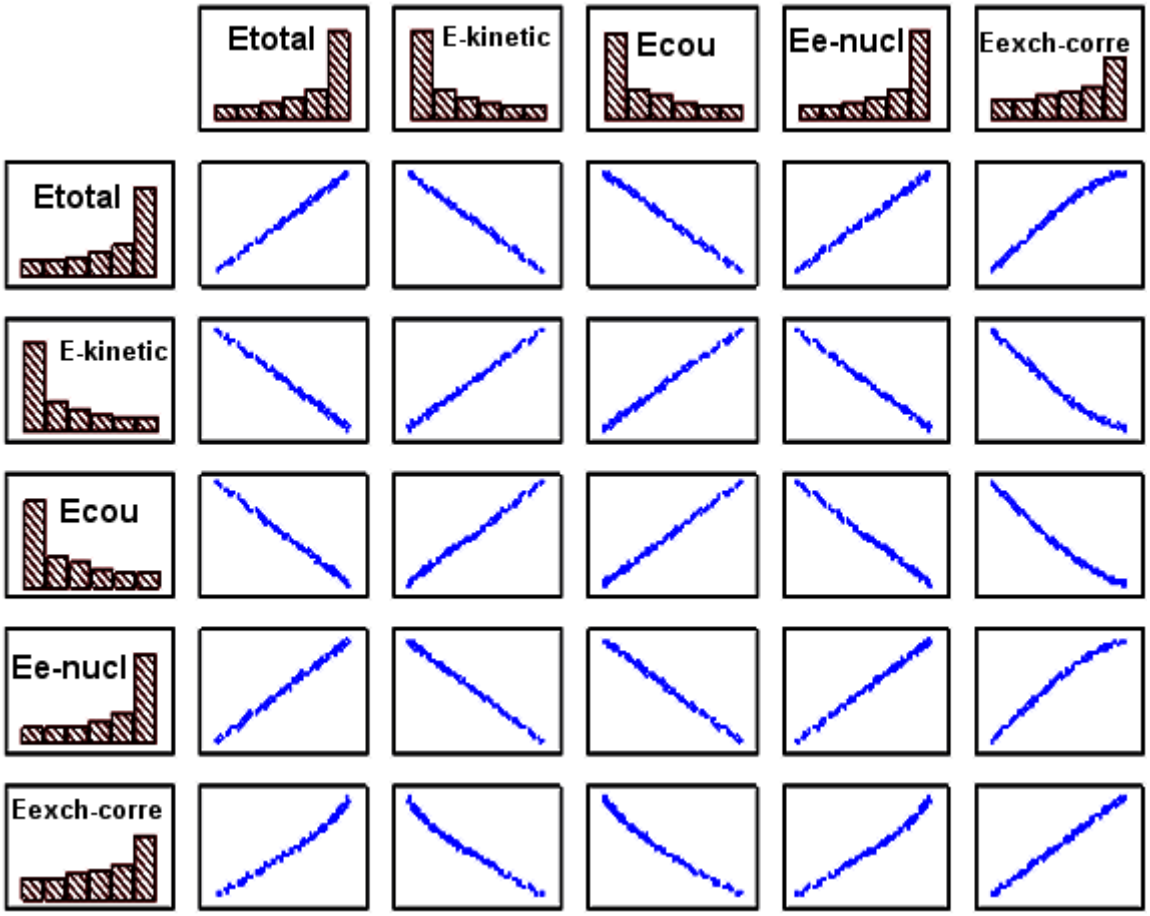

Figure 4

Correlation Matrix of energies

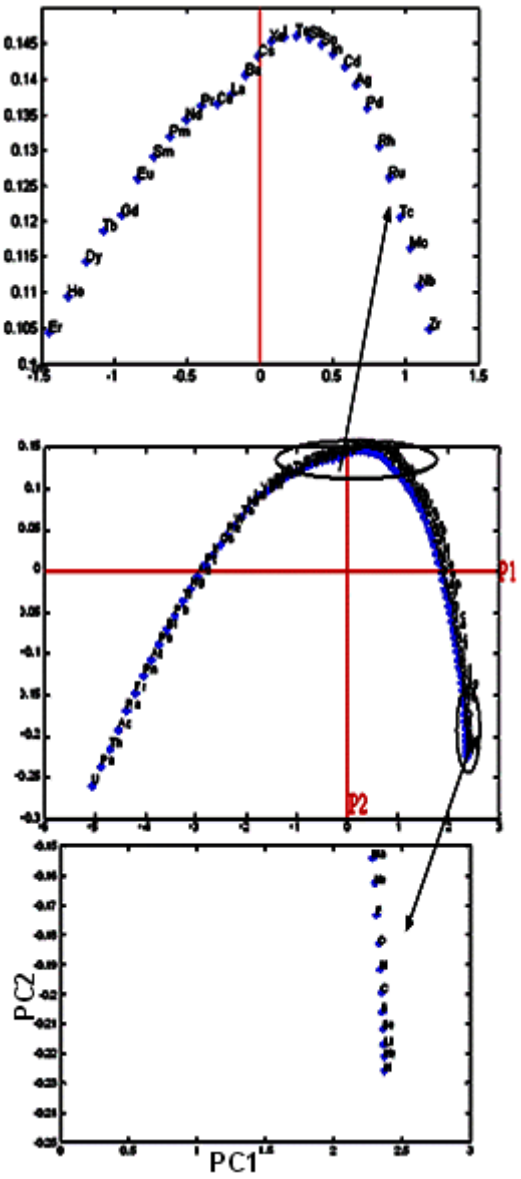

Figure 5

The correlation between elements - Loading plot

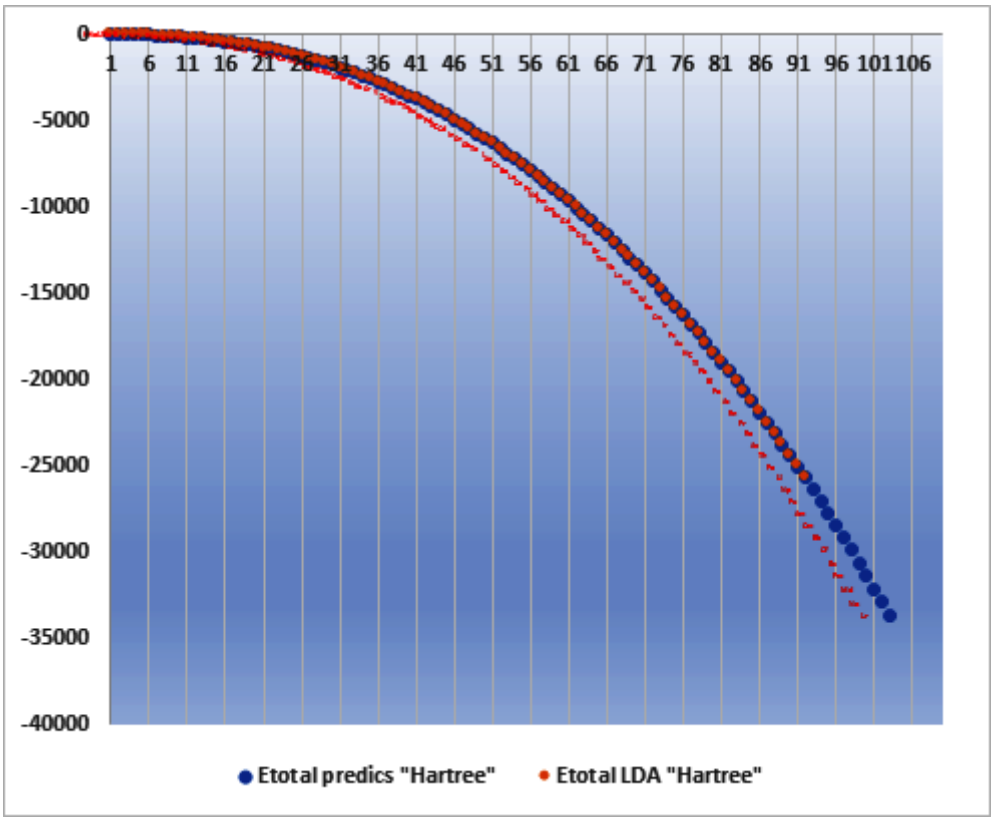

Figure 6

polynomial of total atomic energy