# Quantum mechanical investigation of iron nanoparticle and its nanocomposites

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## Abstract

In this work, the theoretical visual models were constructed for iron nanoparticle and its nanocomposites. These models have been investigated by Hartree-Fock-Roothaan (HFR) method. Molecular orbitals are represented as blend in a linear combination of atomic orbitals of the atoms of the iron nanoparticle and its nanocomposites. It has been used as atomic orbitals whoever ; atomic iron orbitals Fe : 1s-, 2s-, $2p_x$-, $2p_y$-, $2p_z$-, 3s-, $3p_x$-, $3p_y$-, $3p_z$-, $3d_x^2$-, $3d_y^2$-, $3d_z^2$-,$3d_{xy}$-, $3d_{xz}$-, $3d_{yz}$-, 4s-, $4p_x$-, $4p_y$-, $4p_z$- and, 1s-, 2s-, $2p_x$-, $2p_y$-, $2p_z$- are atomic orbitals of Carboon (C) and floure (F), also 1s- atomic orbitals of Hydrogen (H).

Besides, Gaussian functions have been used as atomic orbitals. The numerical values of unknown coefficients of the linear combination have been found from the solution of HFR equations. As a result of this calculations, the values of orbital energies, ionization potential, and the total electronic energy of iron nanoparticle and its nanocomposites have been determined . The calculations show that iron nanoparticle and polyvinliden floride + $iron_8$ (PVDF+$Fe_8$) nanocomposite are tough, electrophile, and stable dielectric, and polypropylene + $iron_8$(PP+$Fe_8$ )is tough, nucleophile, and stable semi-conductive material. The effective charge of atoms have been calculated and molecular diagrams of iron nanoparticles and its nanocomposites have been constructed.

**Key words:** nanotechnology, quantum-mechanical calculation, computer models Hartree – Fock – Roothaan method.

### Introduction and theoretical methodology

Iron nanoparticle is used in a large field of electronics and medicine devices . For this reason, it has a great importance to investigate electronic structure of iron nanoparticle and its nanocomposites by quantum mechanical methods [1, 8, 9]. In the given work, electronic structure and properties of iron nanoparticle and its nanocomposites have been studied by Hartree-Fock-Roothaan (HFR) method. As HFR method, the state of electron in the molecule is represented with one-electronic wave functions called $U_i$– molecular orbitals. $U_i$ is represented as linear combinations of $\mathcal{X}_q$ atomic orbitals of atoms of molecules [4, 7], with :

$$U_i = \sum_q c_{qi}\mathcal{X}_q \qquad (1)$$

$\mathcal{X}_q$ orbitals are considered as known. Unknown coefficients $C_{qi}$ are found from the solution of HFR equations. We can express these equations in matrix form as following:

$$FC=\varepsilon SC \qquad (2)$$

Here, ε- orbital energies of electrons, S- overlap matrix elements between $\mathcal{X}_P$ and $\mathcal{X}_q$ atomic orbitals, C- matrix of unknown coefficients. F is matrix elements of Fock operator, it depends on the C unknown coefficients. By unitary conversion method (2) ,it is possible to converse generalized eigenvalues equations to ordinary eigenvalues equations. As a result of calculations, $\varepsilon_i$- orbital energies, and values of coefficients $C_{qi}$ have been found. On basis of values of coefficients $C_{qi}$ the analytical expression of molecular orbitals can be obtained. This allows to calculate some parameters of nanostructures, such as effective charge of atoms. On basis of the values of $\varepsilon_i$ it is possible to calculate the total energy, the values of ionization potential, electric conductivity, strength, and other properties of iron nanoparticle and its PP+$Fe_8$, PVDF+$Fe_8$ nanocomposites. During calculations as $\mathcal{X}_q$ atomic orbitals, 1s-, 2s-, $2p_x$-, $2p_y$-, $2p_z$-, 3s-, $3p_x$-, $3p_y$-, $3p_z$-, $3d_x^2$-, $3d_y^2$-, $3d_z^2$-,$3d_{xy}$-, $3d_{xz}$-, $3d_{yz}$-, 4s-,

$4p_x$-, $4p_y$-, $4p_z$- atomic orbitals of Fe, 1s-, 2s-, $2p_x$-, $2p_y$-, $2p_z$- atomic orbitals of C and F, and 1s- atomic orbitals of H have been used.Gaussian functions have been used as atomic orbitals.

## Result and Discussion:

### Computer calculations for ($Fe_8$) nanoparticle :

Initially, ($Fe_8$) nanoparticles have been investigated.It is known that the structure and properties of nanoparticles, are defined by the number of atoms and geometrical dimensions of nanoparticle. The dimension of nanoparticle composed with N same type of atoms is defined by the following formula [2, 3, 11, 12, 13]:

$$D = \sqrt[3]{\frac{6MN}{\pi\rho N_A}} \qquad (3)$$

Here, M is – molar mass of atoms, ρ-is material density, and $N_A$- is Avogadro's number. By calculating dimension of nanoparticle composed with N=8 iron atoms by formula (3) we get D= 0,565nm. During calculations, 152 atomic orbitals (19 of each Fe atom) have been used. On the basis of formula (1) 152 molecular orbitals have been constructed. 26*8=208 of electrons of nanoparticle occupy the lowest 104 energy levels. In Fig. (1). The selected spatial structure for $Fe_8$ has been given[5, 6, 10].

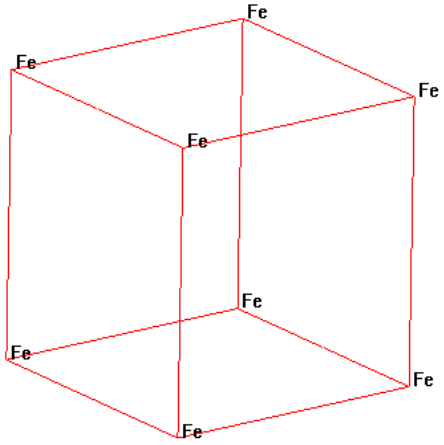


Fig. (1).

The result of calculations have been given below:
Total energy = -10171.418094282 (a.u.)
Kinetic energy of electrons = 9900.661386989 (a.u.)
Virial condition (-V/T) =2.0273
Orbital energies (eV)

Table (1) : orbital energies (eV) of ($Fe_8$)

| | | | | | |
|---|---|---|---|---|---|
| -7096.822568 | -7096.819946 | -7096.817610 | -7096.816063 | -7037.931405 | -7037.930384 |
| -7037.930207 | -7037.927937 | -910.637665 | -910.636656 | -910.626172 | -910.612197 |
| -853.130185 | -853.128607 | -853.116597 | -853.105148 | -799.317574 | -799.316197 |
| -799.314152 | -799.311581 | -799.121493 | -799.121025 | -799.118341 | -799.116113 |
| -799.106677 | -799.105782 | -799.103343 | -799.101098 | -741.887906 | -741.886117 |
| -741.884573 | -741.884021 | -741.824755 | -741.823175 | -741.822597 | -741.822008 |
| -740.833160 | -740.832024 | -740.830779 | -740.830076 | -158.532057 | -154.917343 |
| -154.799356 | -154.793870 | -138.801590 | -138.793314 | -138.792593 | -138.772793 |
| -128.778788 | -128.748059 | -128.558175 | -128.555449 | -94.436589 | -94.389907 |
| -94.389377 | -94.309305 | -94.221097 | -94.105926 | -94.105534 | -94.058233 |
| -93.671868 | -93.333124 | -93.332137 | -93.147751 | -92.406785 | -92.324305 |
| -92.195689 | -92.195005 | -90.307362 | -90.286068 | -90.285576 | -90.277253 |

| | | | | | |
|---|---|---|---|---|---|
| -86.023001 | -85.909928 | -85.907766 | -85.882359 | -67.883421 | -67.832601 |
| -66.561125 | -66.556794 | -64.061908 | -64.058788 | -63.681253 | -61.746873 |
| -33.424035 | -26.206456 | -26.204183 | -24.916063 | -24.727969 | -24.153146 |
| -24.151216 | -22.043344 | -22.015108 | -21.879577 | -21.837397 | -21.836590 |
| -21.679444 | -21.318306 | -21.317703 | -20.286774 | -19.738143 | -19.425773 |
| -19.423550 | -12.686415 | -7.131742 | -7.131573 | -5.807887 | -4.173463 |
| -2.055968 | -1.893116 | -1.892549 | -1.771761 | -1.562196 | -0.453927 |
| -0.112676 | -0.112317 | 0.257151 | 0.399862 | 0.539088 | 0.540170 |
| 0.558914 | 0.616605 | 0.616663 | 1.022404 | 1.169800 | 1.905328 |
| 1.906549 | 2.105872 | 10.416848 | 17.640306 | 17.643119 | 29.083910 |
| 46.950301 | 49.127849 | 51.122128 | 51.125896 | 66.504896 | 66.777966 |
| 71.931227 | 71.932470 | 77.521887 | 77.523312 | 82.445601 | 83.470483 |
| 83.541986 | 87.487192 | 87.489059 | 90.703296 | 154.089378 | 163.030894 |
| 163.030969 | 179.241648 | | | | |

Table (2) : The effective charge and coordinates (with Angstrom) of atoms

| No of Atom | Z | Effective charge | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 8.228390 | -1.23908700 | -0.59242850 | 1.06279800 |
| 2 | 26 | 8.228306 | -1.23908700 | 1.74754900 | 1.06279800 |
| 3 | 26 | -8.228249 | 1.10082000 | -0.59242850 | 1.06279800 |
| 4 | 26 | -8.229038 | 1.10094700 | 1.74754900 | 1.06279800 |
| 5 | 26 | -8.228307 | 1.10082000 | -0.59242850 | -1.27725700 |
| 6 | 26 | 8.228543 | -1.23908700 | -0.59242850 | -1.27719800 |
| 7 | 26 | -8.228143 | 1.10082000 | 1.74747000 | -1.27725700 |
| 8 | 26 | 8.228501 | -1.23908700 | 1.74765800 | -1.27719800 |

**Interpretation of the results for ($Fe_8$) nanoparticle:**

208 electrons of ($Fe_8$)nanoparticle have been located at two by two levels starting from the lowest energy level. The value of band gap can be calculated as $E_g = \varepsilon_{LUMO} - \varepsilon_{HOMO}$. Here, $\varepsilon_{LUMO}$ is the energy of the lowest empty molecular orbital, and $\varepsilon_{HOMO}$is the highest energy of molecular orbital occupied by electrons.

$\varepsilon_{LUMO} = \varepsilon_{105} = -7.131742\ eV$,$\varepsilon_{HOMO} = \varepsilon_{104} = -12.686415eV$,

$\varepsilon_{LUMO} - \varepsilon_{HOMO} = \varepsilon_{105-}\varepsilon_{104} = -7.131742 - (-12.686415) = 5.554673eV$.

And this shows that $Fe_8$ nanoparticle is dielectrical material. The energy of the highest level occupied by electrons is equal to the value of ionization potential with negative sign.

$I_p = -\varepsilon_{HOMO} = -\varepsilon_{104} = 12.686415\ eV$ [4]. Strength can be calculated by the formula: $\eta = \frac{1}{2}(\varepsilon_{LUMO} - \varepsilon_{HOMO})$. Consequently, as $\eta = 2.7773365eV$, $\eta < 1eV$, $Fe_8$ nanoparticle considered as tough material. $Fe_8$nanoparticleis electrophile, as $\varepsilon_{LUMO}$ is negative sign. The stability of $Fe_8$ nanoparticle is calculated by formula:

$\Delta E(Fe_8) = E_{Fe_8} - 4 \cdot E_{Fe_2}$.

When $\Delta E(Fe_8) > 0$, the material is considered unstable and when $\Delta E(Fe_8) < 0$, the material is considered stable. $E_{Fe_8}$is the calculated total energy of $Fe_8$ nanoparticle and $E_{Fe_2}$is the calculated total energy of $Fe_2$ nanoparticle.

As$E_{Fe_8} = -10171.41809\ a.u.$,

$E_{Fe_2} = -2513.261434\ a.u.\ \Delta E(Fe_8) = -118.3723601\ a.u.$,

$Fe_8$ nanoparticle is stable, because$\Delta E(Fe_8) < 0$.

## Computer calculations for (PP+$Fe_8$) nanocomposite:

$Fe_8$nanocomposites located between two $C_3H_6$ polymers have been considered as visual model of PP+$Fe_8$ nanocomposite. During calculations, 194 basis functions (5 of each C atom, 1 of each H atom,

and 19 of each Fe atom) have been used. 256 electrons of nanocomposite fill the lowest 128 energy levels. In Fig.(2), aselected spatial structure of theoretical model for PP+$Fe_8$ nanocomposite has been given.

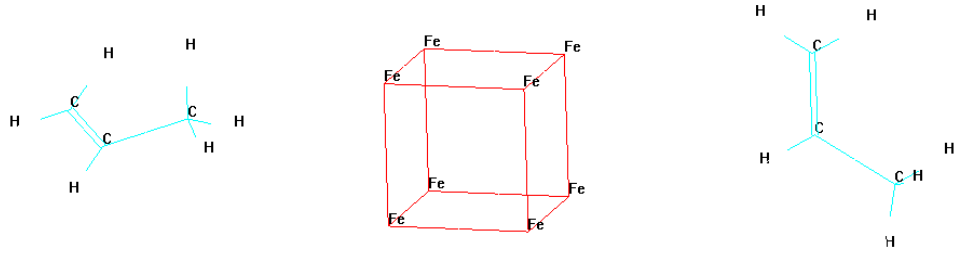


Fig. (2) . (PP+$Fe_8$) nanocomposite

The result of calculations for (PP+$Fe_8$) nanocomposite have been given below:

Total energy = -11051.24584 (a.u.)

Kinetic energy of electrons = 10132.206526127 (a.u.)

Virial condition (-V/T) = 2.0907

ORBITAL ENERGIES (Ev)

Table (3) : Orbital energies (eV) of (PP +$Fe_8$) nanocomposites

| | | | | |
|---|---|---|---|---|
| -7071.684572 | -7069.824261 | -7064.544964 | -7063.254774 | -7026.751775 |
| -7025.381067 | -7022.331861 | -7022.275150 | -885.680514 | -883.801935 |
| -878.509915 | -877.204965 | -841.941295 | -840.625271 | -837.516662 |
| -837.452798 | -789.287770 | -774.713327 | -773.991150 | -773.981239 |
| -772.865305 | -772.128644 | -772.064047 | -767.811638 | -766.726061 |
| -766.699704 | -766.502907 | -765.416627 | -765.400831 | -730.847482 |
| -730.273672 | -730.131409 | -729.507331 | -728.947167 | -728.793502 |
| -726.472639 | -726.429122 | -725.883658 | -725.796654 | -725.584123 |
| -725.518826 | -705.835663 | -684.897416 | -586.941454 | -546.615612 |
| -541.990085 | -535.951328 | -531.080541 | -524.700055 | -488.882301 |
| -470.525133 | -437.992397 | -413.229569 | -394.508068 | -334.308803 |
| -311.194338 | -291.342062 | -279.711490 | -262.061449 | -254.423770 |
| -241.305084 | -124.984493 | -121.616491 | -121.187645 | -119.046721 |
| -118.347707 | -116.747561 | -114.030092 | -112.772470 | -108.992347 |
| -107.997512 | -107.615801 | -107.110716 | -75.946733 | -75.397400 |
| -75.158334 | -75.055729 | -74.909195 | -74.835256 | -74.473883 |
| -73.782600 | -73.617894 | -73.575255 | -73.504857 | -73.324335 |
| -72.141482 | -71.553405 | -71.316306 | -71.160517 | -70.606026 |
| -70.286833 | -70.264365 | -70.023832 | -69.299971 | -68.683308 |
| -68.633010 | -67.829504 | -47.607809 | -46.534290 | -46.368431 |
| -45.785920 | -44.430602 | -43.077596 | -42.786373 | -42.034966 |
| -29.986635 | -15.568177 | -10.027821 | -9.476326 | -8.531026 |
| -7.870093 | -7.829176 | -7.682390 | -7.094917 | -6.746170 |
| -6.415272 | -6.205550 | -5.822196 | -5.522025 | -5.098737 |
| -4.173257 | -3.965915 | -3.828429 | -2.481598 | -2.168111 |
| -1.075205 | -0.395117 | -0.116930 | 2.564777 | 5.324675 |
| 12.780643 | 14.980746 | 16.861847 | 17.131503 | 17.241097 |
| 17.310159 | 17.794194 | 18.344158 | 18.729016 | 18.757126 |
| 19.121965 | 19.425054 | 19.664006 | 19.843318 | 20.237129 |
| 20.341468 | 20.836695 | 21.251155 | 21.683650 | 21.841910 |
| 22.185508 | 24.219948 | 30.796039 | 30.864521 | 42.058923 |

| | | | | |
|---|---|---|---|---|
| 65.043910 | 66.050166 | 68.054764 | 68.162289 | 68.680377 |
| 70.155667 | 73.867556 | 75.055929 | 75.418358 | 79.225087 |
| 80.783234 | 86.180653 | 86.811701 | 94.283685 | 97.566417 |
| 98.065996 | 99.879278 | 136.228042 | 146.625588 | 152.333701 |
| 165.834372 | 270.938169 | 285.997346 | 293.304616 | 309.434183 |
| 325.433800 | 329.783345 | 348.440795 | 352.519363 | 354.751741 |
| 379.660565 | 407.796970 | 452.592242 | 459.813472 | 508.959343 |
| 511.993905 | 512.115902 | 594.332452 | 598.282888 | |

Table (4) : The effective charge and coordinates (with Angstrom) of atoms

| No of Atom | Z | Effective Charge | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 6.704114 | -1.23910832 | -0.59237454 | -1.27722725 |
| 2 | 26 | -7.848253 | 1.10086245 | -0.59250094 | -1.27722725 |
| 3 | 26 | 6.729828 | -1.23910832 | 1.74753304 | -1.27722725 |
| 4 | 26 | -7.851104 | 1.10086245 | 1.74753304 | -1.27722725 |
| 5 | 26 | 7.786721 | -1.23910832 | 1.74753304 | 1.06282733 |
| 6 | 26 | 7.388113 | -1.23910832 | -0.59237454 | 1.06276816 |
| 7 | 26 | -7.390213 | 1.10079035 | 1.74753304 | 1.06282733 |
| 8 | 26 | -7.518702 | 1.10097803 | -0.59237454 | 1.06276816 |
| 13 | 6 | -3.999999 | 6.87297390 | 0.48424481 | -0.67000387 |
| 14 | 6 | -4.000002 | 6.04788391 | 0.80795842 | 0.33500160 |
| 15 | 6 | -4.000019 | 4.61481221 | 0.30129728 | 0.33500160 |
| 18 | 6 | 3.999345 | -5.27093976 | -0.66931905 | -1.66616999 |
| 19 | 6 | 4.000217 | -5.27093976 | 0.67068095 | -1.66616999 |
| 20 | 6 | 5.999555 | -6.58729837 | 1.43068095 | -1.66616999 |
| 11 | 1 | -1.000000 | 7.89120905 | 0.84424089 | -0.67000387 |
| 16 | 1 | -1.000000 | 6.51973665 | -0.13665478 | -1.48000828 |

**Interpretation of the results for (PP+$Fe_8$) nanocomposite:**

The value of ionization potential of (PP+$Fe_8$) nanocomposite is calculated by: $I_p = \varepsilon_{128} = 0.11693\ eV$. Value of the band gap is:

$E_g = \varepsilon_{LUMO} - \varepsilon_{HOMO} = \varepsilon_{129} - \varepsilon_{128} = 2.564777 - (-0.11693) = 2.681707\ eV$.

This shows that (PP+$Fe_8$) nanocomposite is semi-conductive material. Strength is calculated by the formula:

$\eta = \frac{1}{2}(\varepsilon_{LUMO} - \varepsilon_{HOMO})$. $\varepsilon_{LUMO} = \varepsilon_{129} = 2.564777eV$. $\varepsilon_{HOMO} = \varepsilon_{128} = -0.11693eV$.

Consequently, as $\eta = 1.3408535eV$, $\eta < 1eV$, (PP+$Fe_8$) nanocomposite is considered tough material. (PP+$Fe_8$) nanocomposite is nucleophile, as $\varepsilon_{LUMO}$ is positive sign.

The stability of (PP+$Fe_8$) nanocomposite is calculated by the formula:

$\Delta E(PP + Fe_8) = E_{PP+Fe_8} - 4 \cdot E_{Fe_2} - 3E_{C_2} - 6E_{H_2}$.

$E_{PP+Fe_8}$ is the total energy of PP+$Fe_8$ nanocomposite,

$E_{Fe_2}$ is total energy of $Fe_2$, $E_{C_2}$ is the total energy of $C_2$ , and $E_{H_2}$ is the total energy of $H_2$.

As $E_{PP+Fe_8} = -11051.24584\ a.u.$, $E_{Fe_2} = -2513.261434\ a.u.$, $E_{C_2} = -74.31543142\ a.u.$, $E_{H_2} = 1.111298185\ a.u.$, $\Delta E(PP + Fe_8) = -768.5860176\ a.u.$ (PP+$Fe_8$), nanocomposite is stable because $\Delta E(PP + Fe_8) < 0$.

**Computer calculations for (PVDF+$Fe_8$) nanocomposite**

$Fe_8$ nanoparticle located between two $C_2H_2F_2$ have been considered as theoretical model of (PVDF+$Fe_8$) nanocomposites, During calculations, 196 basis functions (5 of each C and F atoms, 1 of each H atom, and 19 of each Fe atom) have been used and 196 molecular orbitals have been constructed. 272 electrons of nanocomposite fill the lowest 136 energy levels. In Fig. (3) .

The selected spatial structure of theoretical model for(PVDF+$Fe_8$)nanocomposite has been given

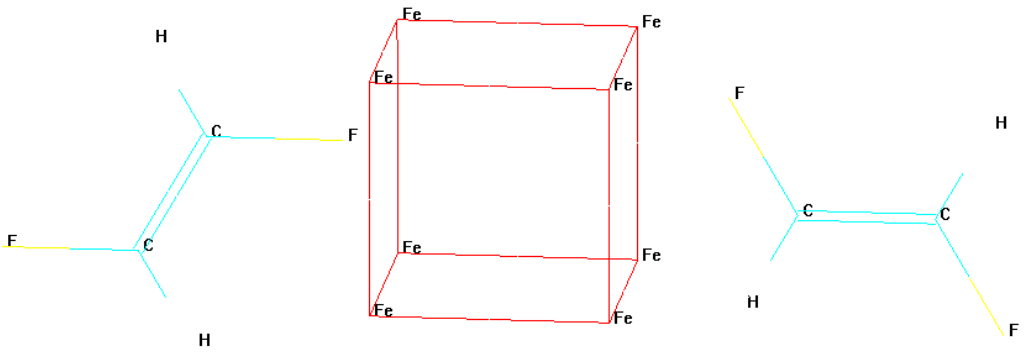


Fig. (3) . (PVDF+$Fe_8$ ) nanocomposites

The result of calculations for (PVDF+$Fe_8$) nanocomposite have been given as follows :
Total energy = -10742.095170728 (a.u.)
Kinetic energy of electrons = 10452.694306077 (a.u.)
Virial condition (-V/T) = 2.0277

Table (5) Orbital ebergies (eV) of (PVDF+$Fe_8$ ) nanocomposites

| | | | | |
|---|---|---|---|---|
| -7112.924390 | -7110.342971 | -7106.041309 | -7104.967173 | -7059.501851 |
| -7054.131629 | -7048.256263 | -7047.989609 | -926.741329 | -924.162516 |
| -920.281365 | -919.109019 | -874.961422 | -869.287727 | -863.359797 |
| -863.137744 | -815.311258 | -815.284158 | -815.268029 | -813.110205 |
| -812.789667 | -812.682210 | -812.655555 | -808.926200 | -808.711785 |
| -808.684364 | -807.740988 | -807.573387 | -807.495132 | -763.518601 |
| -763.401467 | -763.250695 | -758.296392 | -757.553299 | -757.394252 |
| -756.922776 | -752.164976 | -752.060774 | -751.888434 | -751.484531 |
| -751.364080 | -751.190088 | -750.201342 | -741.770546 | -335.298896 |
| -323.835771 | -319.761622 | -319.425505 | -180.300686 | -159.182352 |
| -157.553978 | -156.681796 | -155.976736 | -153.544110 | -151.907073 |
| -151.237194 | -150.523688 | -147.920234 | -141.363858 | -139.065502 |
| -135.790914 | -135.569258 | -134.814864 | -134.483509 | -122.452890 |
| -118.449258 | -108.781213 | -108.688541 | -107.703067 | -107.546704 |
| -107.345918 | -107.238617 | -107.111455 | -106.804335 | -105.952750 |
| -105.509246 | -105.425823 | -104.813965 | -104.569449 | -103.083676 |
| -102.827034 | -102.691352 | -101.274691 | -100.387718 | -100.182585 |
| -100.120751 | -99.317402 | -98.857210 | -94.645517 | -94.522135 |
| -88.643123 | -87.163150 | -79.423840 | -75.181262 | -74.491118 |
| -73.858854 | -72.200898 | -71.091964 | -70.091494 | -69.525880 |
| -68.631885 | -67.732782 | -67.137951 | -65.245396 | -63.374306 |
| -62.425968 | -59.850626 | -57.010089 | -52.218037 | -50.261826 |
| -49.709450 | -44.874428 | -42.499137 | -42.119433 | -40.168553 |
| -39.721665 | -39.125737 | -38.284716 | -38.005533 | -36.943309 |
| -36.648214 | -34.933515 | -34.215977 | -33.623384 | -32.772601 |
| -32.645790 | -32.212537 | -31.862347 | -31.050990 | -30.729521 |
| -30.325570 | -29.675598 | -28.391376 | -27.390998 | -26.762508 |
| -24.101256 | -19.455838 | -19.053461 | -18.346847 | -17.510036 |
| -17.099354 | -16.505540 | -15.043854 | -14.651794 | -14.110454 |

| | | | | |
|---|---|---|---|---|
| -13.883078 | -13.666890 | -13.621725 | -13.169202 | -12.861181 |
| -12.587159 | -12.315206 | -11.667658 | -11.377430 | -11.262104 |
| -10.852828 | -10.720603 | -10.196712 | -9.681988 | -9.348315 |
| -9.276863 | -8.452905 | -8.302233 | -7.414309 | -6.332402 |
| -5.190824 | -3.197342 | -0.375265 | 0.717470 | 2.560503 |
| 7.790112 | 8.773945 | 9.449914 | 22.380734 | 38.579006 |
| 41.224930 | 43.636207 | 43.845308 | 55.722993 | 57.829262 |
| 59.437901 | 63.607569 | 65.765091 | 69.607534 | 72.536355 |
| 72.968606 | 73.436549 | 76.241551 | 76.662357 | 80.139674 |
| 82.506273 | 87.026726 | 145.985269 | 154.354024 | 155.943419 |
| 170.121132 | | | | |

Table (6) : The effective charge and coordinates (with Angstrom) of atoms

| No of Atom | Z | Effective charge | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 7.661104 | -1.23908721 | -0.59242849 | 1.06279775 |
| 2 | 26 | 7.844495 | -1.23908721 | 1.74754897 | 1.06279775 |
| 3 | 26 | -7.278534 | 1.10082036 | -0.59242849 | 1.06279775 |
| 4 | 26 | -7.135825 | 1.10094677 | 1.74754897 | 1.06279775 |
| 5 | 26 | -7.683772 | 1.10082036 | -0.59242849 | -1.27725683 |
| 6 | 26 | 8.175063 | -1.23908721 | -0.59242849 | -1.27719766 |
| 7 | 26 | -7.915455 | 1.10082036 | 1.74747018 | -1.27725683 |
| 8 | 26 | 8.401979 | -1.23908721 | 1.74765785 | -1.27719766 |
| 9 | 6 | -0.932745 | 0.42866191 | -3.57436400 | 0.39854940 |
| 10 | 6 | -0.406608 | 0.42866191 | -2.23436400 | 0.39854940 |
| 11 | 9 | 1.735796 | -0.72315187 | -1.56936400 | 0.39854940 |
| 12 | 9 | -1.004532 | 1.58047570 | -4.23936400 | 0.39854940 |
| 15 | 9 | -0.125206 | -0.09164610 | 2.24624800 | 0.77426600 |
| 16 | 6 | -3.249944 | 1.06882794 | 4.24624800 | 0.77426600 |
| 17 | 6 | 2.840179 | -0.09164610 | 3.57624800 | 0.77426600 |
| 18 | 9 | -0.995179 | 1.06882794 | 5.57624800 | 0.77426600 |
| 13 | 1 | 1.018749 | -0.50664552 | -4.11436400 | 0.39854940 |
| 14 | 1 | -0.951997 | 1.36396935 | -1.69436400 | 0.39854940 |
| 19 | 1 | 0.999348 | -1.02695354 | 4.11624800 | 0.77426600 |
| 20 | 1 | -0.996907 | 2.00413537 | 3.70624800 | 0.77426600 |

**Interpretation of the results for (PVDF+$Fe_8$) nanocomposite:**

The value of ionization potential of (PVDF+$Fe_8$ ) nanocomposites: $I_p = -\varepsilon_{136} = 24.101256\, eV$. Value of the band gap is:

$E_g = \varepsilon_{LUMO} - \varepsilon_{HOMO} = \varepsilon_{137} - \varepsilon_{136} = -19.455838 - (-24.101256) = 4.645418\, eV$.

And this shows that (PVDF+$Fe_8$) nanocomposites is dielectrical material. Strength is calculated by the formula:

$\eta = \frac{1}{2}(\varepsilon_{LUMO} - \varepsilon_{HOMO})$.

Here, $\varepsilon_{LUMO} = \varepsilon_{137} = -19.455839eV$. $\varepsilon_{HOMO} = \varepsilon_{136} = -19.455938eV$.

As $\eta > 1eV$, PVDF+$Fe_8$, nanocomposites is considered tough material. (PVDF+$Fe_8$) nanocomposites is electrophile, as $\varepsilon_{LUMO}$ is negative sign. The stability of nanocomposite is calculated by the formula:

$\Delta E(PVDF + Fe_8) = E_{PVDF+Fe_8} - 4 \cdot E_{Fe_2} - 3E_{C_2} - 6E_{H_2} - 2E_{F_2}$. $E_{PVDF+Fe_8}$is the total energy of (PVDF+$Fe_8$) nanocomposites, $E_{Fe_2}$ is the total energy of $Fe_2$ , $E_{H_2}$is the total energy of $H_2$, $and\ E_{F_2}$ is the total energy of $F_2$.

As $E_{PVDF+Fe_8} = -10742.095170728\ a.u.$, $E_{Fe_2} = -2513.261434\ a.u.$, $E_{C_2} = -74.31543142\ a.u.$, $E_{H_2} = 1.111298185\ a.u.$, $\Delta E(PVDF + Fe_8) = -146.277337\ a.u.$(PVDF+$Fe_8$) nanocomposite is stable because $\Delta E(PVDF + Fe_8) < 0$.

By using the values of coefficient $C_{qi}$ , effective charges of atoms of nanoparticles have been calculated,and the molecular diagrams of ($Fe_8$) nanocomposite, (PP+$Fe_8$) nanocomposites and (PVDF+$Fe_8$) nanocomposites have been constructed. The values of bond length in diagrams are given with Angstrom Fig. (4-6).

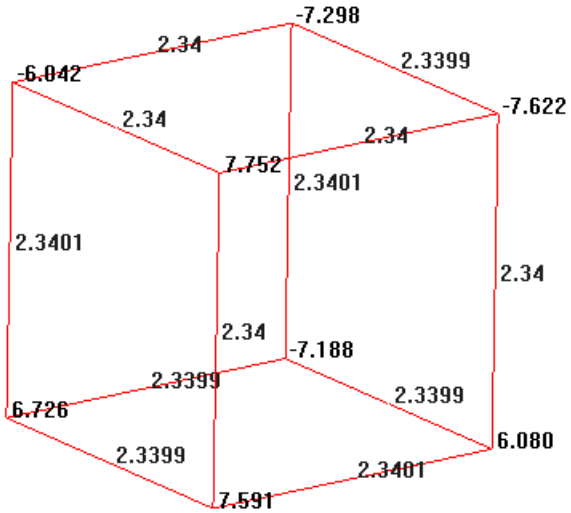


Fig. (4). Molecular diagram of ($Fe_8$) nanocomposite

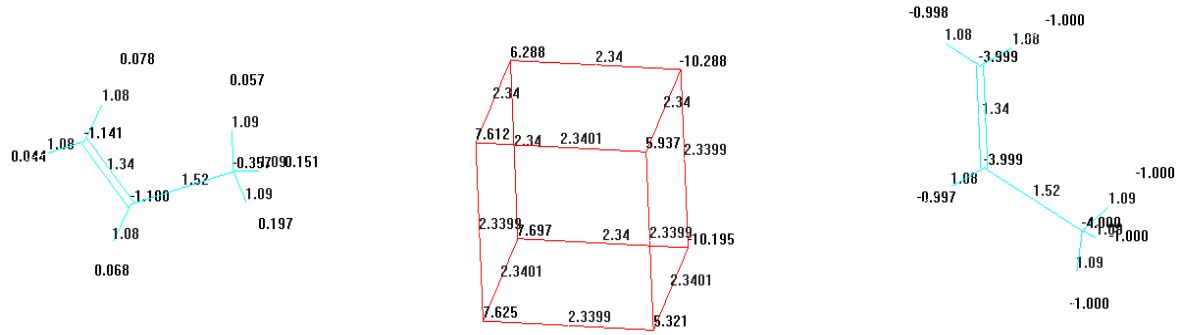


Fig. (5). Molecular diagram of (PP+$Fe_8$) nanocomposite

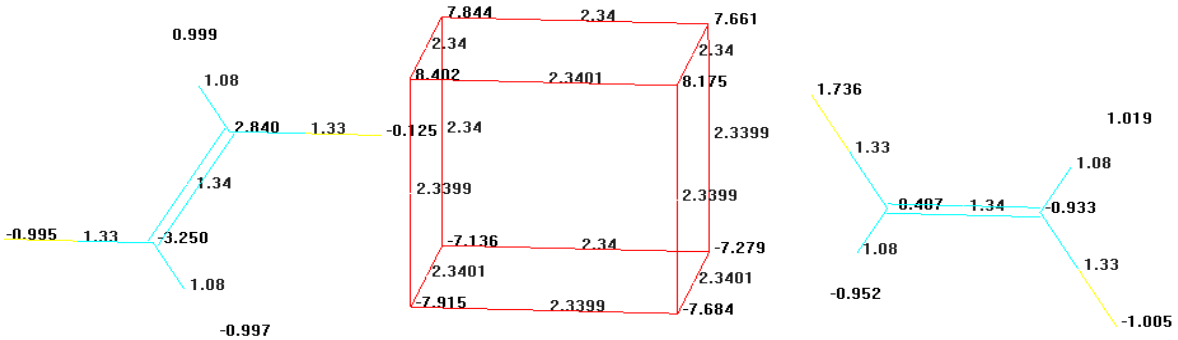


Fig. (6). Molecular diagram of (PVDF+$Fe_8$) nanocomposite

## Conclusion

Iron nanoparticle and its (PP+$Fe_{8,}$ ) and (PVDF+$Fe_8$) nanocompositions have been investigated by HFR method. Orbital energies, ionization potential, values of total electron energies, and effective charges of atoms of iron nanoparticle and its nanocompositions have been calculated. The results of calculations show that iron nanoparticle and (PVDF+$Fe_8$) nanocomposites are tough, electrophile and stable dielectric,(PP+$Fe_8$) nanocomposite is tough, nucleophile, and stable semi-conductive materials.

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# تحقيق ميكانيكا الكم لجسيمات الحديد ومركباتها النانوية

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## الملخص

في هذا العمل تم إعداد النماذج البصرية النظرية لجسيمات الحديد ومركباتها النانوية ، وتم التحقق من هذه النماذج بطريقة هارتري – فوك – روتان (**HFR**) ، وتم تمثيل المدارات الجزيئية كمزيج بالتوافق الخطي لمدارات الذرة لجسيمات الحديد ومركباتها النانوية واستخدمت كمدارات ذرية كلاً من مدارات الحديد (**Fe**) الذرية : 1s-, 2s-, $2p_x$-, $2p_y$-, $2p_z$-, 3s-, $3p_x$-, $3p_y$-, $3p_z$-, $3d_x^2$-, $3d_y^2$-, $3d_z^2$-,$3d_{xy}$-, $3d_{xz}$-, $3d_{yz}$-, 4s-, $4p_x$-, $4p_y$-, $4p_z$- ومدارات الكاربون (**C**) والفلور (**F**): 1s-, 2s-, $2p_x$-, $2p_y$-, $2p_z$- ومدارات الهيدروجين (**H**) : 1s- .
إضافة إلى ذلك فقد تم استخدام دوال جاوس كمدارات ذرية أيضاً، بعد ذلك قمنا بإيجاد القيمة العددية للثوابت المجهولة للتوافق الخطي بواسطة حل معادلات (**HFR**) .
وكنتيجة لهذه الحسابات تم حساب قيمة الطاقات المدارية ، وجهد التأين والطاقة الالكترونية الكلية لجسيمات الحديد ومركباتها النانوية ، حيث أظهرت هذه الحسابات أن جسيمات الحديد النانوية والتركيب النانوي لها (بولي فينيلدن فلورايد + حديد8 (**$PVDF+Fe_8$**) تكون: متينة (صلبة) وجاذبة للإلكترونات (إلكتروفيل) ومستقرة وعازلة كهربائياً.
ومركبات الحديد (بولي بروبلين +حديد 8) (**$PP+Fe_8$**) تكون: متينة (صلبة) وجاذبة للأنوية أو مانحة للألكترونات (نيوكلوفيل) ومستقرة ومادة شبه موصلة.
وكذلك تم حساب الشحنة الفعالة (التأثيرية) للذرات، وتم إعداد النماذج الجزيئية لجسيمات الحديد ومركباتها النانوية.

**الكلمات المفتاحية:** تقنيات النانو (النانوتكنولوجيا)، حساب ميكانيكا الكم ،النماذج الحاسوبية ، طريقة هارتري – فوك – روتان.