ORIENTAL JOURNAL OF CHEMISTRY
An International Open Free Access, Peer Reviewed Research Journal
www.orientjchem.org
Est. 1984
ISSN: 0970-020 X
CODEN: OJCHEG
2015, Vol. 31, No. (3):
Pg. 1515-1536

Theoretical investigation of the zirconium carbide nano-sheet: A study of NMR, NBO, EPR and Polar

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http://dx.doi.org/10.13005/ojc/310330

(Received: June 19,2015; Accepted: July 26, 2015)

ABSTRACT

This study was carried out to investigate the zirconium carbide nano-sheet. Zirconium carbide is one of the metal carbides with unique chemical and physical properties such as high melting point (~3540°C), high hardness (~25 Gpa), wear resistance and high thermal conductivity, and has been shown to have a wide range of applications in various industries. Ab initio methods were carried out for the zirconium carbide nano-sheet using the Gaussian 09 program for the first time. Thus, B3LYP was selected for calculating the natural bond orbital (NBO), Nuclear magnetic resonance (NMR), Electron paramagnetic resonance (EPR) and polar.

Key words: zirconium carbide nano-sheet, NBO, NMR, EPR and polar

INTRODUCTION

The three known allotropes of carbon are amorphous carbon, graphite, and diamond. New allotropes of carbon that are being synthesized around the world include fullerenes, carbon nano tubes (CNTs) and graphene due to their fantastic physical and chemical properties[1-20]. Graphene is a single-atom-thick planar sheet of carbon atoms hexagonally arranged in a honeycomb crystal lattice, and has gained lots of attention due to its structure and electrical properties[21-25]. Graphene is unanimously considered a very promising material to be used in various fields, such as energy production and storage, gas detection, and electronics. In the view of structure, it has one or a few layers thickness of sp^2-hybridized carbon atoms arranged in a honeycomb

pattern, which makes it to possess electrical, optical, electrochemical and mechanical properties. Therefore, several methods for the synthesis of graphene and its derivatives have been developed [26-30]. This study was carried out to explore zirconium carbide nano-sheet (ZrC nano-sheet). ZrC nano-sheet is similar to that of graphene, except that Zr is one among the alternative carbons. Zirconium carbide, due to its unique physical and chemical properties, such as high melting point (~3540°C), high hardness (~25 Gpa), wear resistance, high thermal conductivity, excellent mechanical properties and good chemical stability at high temperature, is used in industries, especially for high temperature applications[31-41]. It is used in different applications such as cutting tools, covering of the tip of the drill, grinding wheels and abrasives for mechanical as well as structural components in chemical and electronic industries. Also, it has potential applications as coating material for nuclear fuel [42-44].

In this study, the molecular mechanic and ab-initio methods were applied to calculate the natural bond orbital (NBO), Nuclear magnetic resonance (NMR), Electron paramagnetic resonance (EPR) and polar of ZrC nano-sheet, using the Gaussian 09 program package.

MATERIALS AND METHODS

Ab initio methods were carried out for the zirconium carbide nano-sheet using the Gaussian 09 program for the first time (Figure 1.). B3LYP was selected for calculating the natural bond orbital (NBO), Nuclear magnetic resonance (NMR), Electron paramagnetic resonance (EPR) and polar.

RESULTS AND DISCUSSION

The E_{HOMO} and E_{LUMO} calculated using the B3LYP method were -0.18646 and -0.16892 (a.u.), respectively. The Band Gap (Fermi energy), Dipole moment, Quadrupole moment, Traceless Quadrupole moment and Octapole moment were calculated using the B3LYP method shown in Table 1.

Table1. Polar determinant and band gap (Fermi energy) obtained for ZrC nano-sheet.

Dipole moment (Debye)	35.215
Quadrupole moment (Debye-Ang)	-64119124.96
Traceless Quadrupole moment (Debye-Ang)	-98480.8764
Octapole moment (Debye-Ang)	-79586.9398
Hexadecapole moment (Debye-Ang)	6.53E+11
Distance matrix (angstrom)	-1.46E+54
Band Gap Energy (a.u.)	-0.01754

Tables 2, 3 and 4 show the calculated parameters of electron paramagnetic resonance (EPR) for ZrC nano-sheet. Atomic bonds, charge of atoms and voltages were determined using the B3LYP method. The ΔV, $\Delta V'$ and ΔV Mulliken for all bonds were calculated.

The formula used given as follow:

$V_1, V_2: \sqrt{X^2+Y^2+Z^2}$, $V_3, V_4: \sqrt{(XX)^2+(YY)^2+(ZZ)^2}$,

V_5,V_6: $\sqrt{(XY)^2+(XZ)^2+(YZ)^2}$, V_9,V_{10}: $\sqrt{X^2+Y^2+Z^2}$,

V_{11},V_{12}: $\sqrt{(3XX-RR)^2+(3YY-RR)^2+(3ZZ-RR)^2}$

$\Delta V' = 27.11\times(V_{first}-V_{second})$, $\Delta V' > 0$

$\Delta V = \frac{K\Delta Q'}{dis\tan ce}$, $\Delta V_{Mulliken}$: $\frac{K\Delta Q}{dis\tan ce}$

Where (V_1,V_2, ΔV_{12} and $\Delta V'_{12}$), (V_5,V_6, ΔV_{56} and $\Delta V'_{56}$) and (V_9,V_{10},ΔV_{910} and $\Delta V'_{910}$) were calculated from the obtained data of EPR that include; (Electrostatic properties “Atomic unit” (X,Y,Z)), (Electric Field Gradient (XY,XZ,YZ)) and (Electric Field Gradient “tensor representation” Eigen values), respectively. Also, (V_{11},V_{12}, ΔV_{1112} and $\Delta V'_{1112}$), (V_3,V_4,ΔV_{34} and $\Delta V'_{34}$) and (V_7,V_8,ΔV_{78} and $\Delta V'_{78}$) were calculated from the obtained data of EPR that include; (Electric Field Gradient “tensor representation” (3XX-RR, 3YY-RR, 3ZZ-RR)), (Electric Field Gradient (XX,YY,ZZ)) and (Electric Field Gradient Eigen values), respectively.

By comparison of the obtained voltages (voltage difference) ; ΔV, $\Delta V'$ and $\Delta V_{Mulliken}$ in Tables 2 and 3 were in similar range, but in Table 4, ΔV and $\Delta V'$ were in a different range of $\Delta V_{Mulliken}$.

The NMR calculated parameters include isotropic shielding tensor (σ_{iso}), anisotropic shielding tensor (σ_{aniso}), asymmetry (η), span (Ω) and skew (K)[45-51].

In this study, the NMR calculated parameters of ZrC nano-sheets obtained using the B3LYP method are shown in Tables 5 to 8.

The equations used are as follows [51]:

$\Omega = \sigma_{33}-\sigma_{11}$, $\xi = \sigma_{33}-\sigma_{iso}$

$\eta = \frac{\sigma_{yy}-\sigma_{xx}}{\xi}$ or $\frac{\sigma_{yy}-\sigma_{zz}}{\xi}$, $0 \le \eta \le 1$

$K = \frac{3(\sigma_{iso}-\sigma_{22})}{\Omega}$, $-1 \le K \le 1$

Where η, Ω, K, ξ were calculated for Zr, H and C, in ZrC nano-sheets. Radii (R) is the distance of He or Ne from ZrC nano-sheets.

Some of the asymmetry in the range $0 \le \eta \le 1$ is not listed in Tables 5-8 and the amount in the table is empty.

Figures 2 and 3 show the diagram of η, σ_{aniso}, σ_{iso}, HF (Hartree-Fock) and K of ZrC nano-sheets with different distance (R) of He and Ne.

Data obtained for natural bond orbital (NBO) are shown in Tables 9 to 15.

E2, Ei- Ej and F (i,j) represent the energy hyper conjugative interaction (stabilization energy), Energy difference between donor and accepter NBO orbital, and the Fock matrix element between i and j orbitals, respectively.

Table 2. EPR calculated parameters for the ZrC nano-sheet.

atomic bond	distance(Å)	$Charge_1$ (a.u.)	$Charge_2$ (a.u.)	V_1 (a.u.)	V_2 (a.u.)	ΔV_{12} (V)	$\Delta V'_{12}$ (V)	V_5 (a.u.)	V_6 (a.u.)	ΔV_{56} (V)	$\Delta V'_{56}$(V)	$\Delta V_{muliken}$ (V)
C1-H26	1.1220	-1.0550	0.2690	1.2974	2.0460	9.6076	20.2945	0.1970	0.7188	6.6960	14.1460	10.0800
C1-H27	1.1220	-1.0550	0.2160	1.2974	2.3320	13.2782	28.0480	0.1970	0.8094	7.8595	16.6022	16.3008
C1-Zr15	2.3100	-1.0550	1.4080	1.2974	0.8530	2.7691	12.0477	0.1970	0.0238	1.0795	4.6955	15.3504
Zr15-C4	2.3100	1.4080	-1.2450	0.8530	0.5958	1.6027	6.9727	0.0238	0.0285	29.2363	0.1274	17.5392
Zr15-C3	2.3100	1.4080	-1.4060	1.2974	1.1972	2.1456	2.7164	0.0238	0.0023	0.1340	0.5829	17.5392
C3-H31	1.1220	-1.4060	0.2390	1.1972	2.5620	17.5147	36.9997	0.0023	0.8328	10.6574	22.5149	21.1104
C3-Zr14	2.3100	-1.4060	1.4180	1.1972	0.7278	2.9260	12.7254	0.0023	0.0064	0.2596	0.1112	17.5968
Zr14-C8	2.3100	1.4180	-1.2890	0.7278	0.1730	3.4574	15.0406	0.0064	0.0065	0.0007	0.0027	16.8624
C8-Zr20	2.3100	-1.2890	1.3290	0.1730	0.3171	0.8971	3.9066	0.0065	0.0018	0.0297	0.1274	16.3152
Zr20-C4	2.3100	1.3290	-1.2450	0.3171	0.5958	1.7366	7.5556	0.0018	0.0284	0.1661	0.7211	16.0416
C4-Zr16	2.3100	-1.2450	0.9640	0.5858	0.9771	2.3760	10.6081	0.0285	0.0422	0.0854	0.3714	13.7664
Zr16-C5	2.3100	0.9640	-0.3520	0.9771	1.3944	2.6006	11.3130	0.0422	1.2071	7.2604	31.5804	8.1936
Zr16-C10	2.3100	0.9640	-0.6460	0.9771	1.4845	3.1622	13.7556	0.0422	0.7175	4.2091	18.3074	10.0224
C10-Zr21	2.3100	-0.6460	0.9290	1.4845	1.1561	2.0462	8.9029	0.7175	0.0275	4.3012	18.7059	9.8064
Zr21-H36	1.8020	0.9290	-0.1740	1.1561	1.8996	5.9400	20.1563	0.0275	0.4489	3.3667	11.4242	8.8128
Zr21-C9	2.3100	0.9290	-1.2370	1.1561	0.6991	2.8483	12.3893	0.0275	0.0153	0.0760	0.3307	13.4928
C9-Zr20	2.3100	-1.2370	1.3290	0.6991	0.3171	4.7332	10.3560	0.0153	0.0018	0.0840	0.3660	15.9840
C9-Zr24	2.3100	-1.2370	1.1200	0.6991	1.0765	2.3515	10.2313	0.0153	0.0169	0.0105	0.0434	14.6880
Zr24-H39	1.8020	1.1200	0.1850	1.0765	1.9784	7.2057	24.4505	0.0170	0.4550	3.4992	11.8742	7.4592
Zr24-C13	2.3100	1.1200	1.2540	1.0765	0.6447	2.6913	11.7061	0.0170	0.0053	0.7270	0.3172	18.2880
C13-Zr19	2.3100	-1.2540	1.3180	0.6447	0.1460	3.1075	13.5198	0.0053	0.0018	0.0216	0.0949	16.0272
C13-Zr23	2.3100	-1.2540	1.0940	0.6447	1.0633	2.6092	11.3482	0.0053	0.0101	0.0299	0.1301	14.6304
Zr23-H38	1.8020	1.0940	-0.1860	1.0633	1.9476	7.0660	23.9734	0.0101	0.4534	3.5409	12.0179	10.2240
Zr23-C12	2.3100	1.0940	-1.2290	1.0633	0.8010	1.6344	7.1110	0.0101	0.1230	0.0135	3.0607	15.3792
C12-Zr22	2.3100	-1.2290	1.2390	0.8010	0.7096	0.5688	2.4779	0.0123	0.0021	13.5115	0.2765	12.3408
C12-Zr25	2.3100	-1.2290	0.7510	0.8010	1.1753	2.9908	10.1473	0.0123	0.1320	0.7459	3.2451	12.3408
Zr25-H41	1.8020	0.7510	-0.1740	1.1753	1.7269	4.4078	14.9539	0.1320	0.0234	0.8668	2.9441	7.3872
Zr25-H43	1.8020	0.7510	0.1890	1.1753	1.7194	4.3473	14.7506	0.1320	0.4076	2.2017	7.4715	4.4784
Zr22-C11	2.3100	1.2390	-0.6580	0.7096	1.3865	4.2192	18.3508	0.0021	0.6281	3.9009	16.9709	15.1488
Zr22-C7	2.3100	1.2390	-1.2690	0.7096	0.3719	2.1033	9.1550	0.0021	0.0271	0.0630	0.6778	15.6240
Zr18-C7	2.3100	1.4430	-1.2690	0.7621	0.3719	2.4321	10.5783	0.0104	0.0271	0.1041	0.4527	16.9056
Zr18-C6	2.3100	1.4430	-1.3240	0.7621	1.2137	2.8137	12.2429	0.0104	0.0732	0.3913	1.7025	17.2368
C6-H33	1.1220	-1.3240	0.2320	1.2137	0.5004	16.4548	19.3376	0.0732	0.8289	9.6984	20.4870	19.9584
C6-Zr17	2.3100	-1.3240	0.8840	1.2137	1.2721	0.3628	1.5832	0.0732	0.0979	0.1540	0.6696	13.7520
Zr17-C11	2.3100	0.8840	-0.6580	1.2721	1.3865	0.7128	3.1014	0.0979	0.6281	3.3033	14.3737	9.6048
C7-Zr19	2.3100	-1.2690	1.3180	0.3719	0.1460	0.1670	6.1241	0.0271	0.0018	0.1569	0.6859	16.1136
Zr19-C8	2.3100	1.3180	-1.2890	0.1460	0.1730	0.1670	0.7320	0.0018	0.0065	0.0295	0.1274	16.2432
Zr14-C8	2.3100	1.4180	-1.2890	0.7278	0.1730	3.4574	15.0406	0.0064	0.0065	7.2311	0.0027	16.8739
Zr14-C2	2.3100	1.4180	-1.4120	0.7278	1.2028	2.9606	12.8773	0.0064	0.0150	0.0532	0.2331	17.6400
C2-H30	1.1220	-1.4120	0.2370	1.2028	0.7278	17.6587	12.8773	0.0150	0.8327	10.4932	22.1678	21.1536
Zr18-C2	2.3100	1.4430	-1.4120	0.7621	1.2028	2.7460	11.9474	0.0104	0.0150	0.0286	0.1247	17.7840

Table 3. EPR calculated parameters for the ZrC nano-sheet.

atomic bond	V_9 (a.u.)	V_{10} (a.u.)	ΔV_{910} (V)	$\Delta V'_{910}$ (V)	V_{11} (a.u.)	V_{12} (a.u.)	ΔV_{1112} (V)	$\Delta V'_{1112}$ (V)
C1-H26	0.5015	1.3454	10.8302	22.8781	0.4169	0.8813	5.9601	12.5899
C1-H27	0.5015	0.2203	10.0598	7.6233	0.4169	0.5749	2.1556	4.2834
C1-Zr15	0.5015	0.5447	0.2692	1.1712	0.4169	0.5436	0.7891	3.4348
Zr15-C4	0.5447	1.2056	4.1198	17.9170	0.5436	1.2049	4.1212	17.9278
Zr15-C3	0.5447	0.6960	0.9417	4.1017	0.5436	0.6959	0.9489	4.1289
C3-H31	0.6960	1.2653	7.3051	15.4337	0.6959	0.4621	2.9995	6.3383
C3-Zr14	0.6960	0.5961	0.6220	2.7083	0.6959	0.5960	0.6220	2.7083
Zr14-C8	0.5961	1.2506	7.4232	17.7435	0.5960	1.2506	4.0795	17.7462
C8-Zr20	1.2506	0.6258	3.8937	16.9383	1.2506	0.6258	3.8938	16.9383
Zr20-C4	0.6258	1.2056	3.6129	15.7184	0.6258	1.2049	3.6086	15.6994
C4-Zr16	1.2056	0.5077	4.3502	18.9201	1.2049	0.5042	4.3675	18.9960
Zr16-C5	0.5077	2.0533	9.6336	41.9012	0.5042	1.1409	3.9686	17.2609
Zr16-C10	0.5077	1.5770	6.6657	28.9887	0.5042	1.2071	4.3804	19.0556
C10-Zr21	1.5770	0.2103	7.5384	37.0512	1.2071	0.3656	5.2444	22.8131
Zr21-H36	0.3676	0.6902	2.5776	8.7457	0.3656	0.2707	0.7574	2.5727
Zr21-C9	0.3676	1.1280	4.7390	20.6144	0.3656	1.1278	4.7505	20.6632
C9-Zr20	1.1280	0.3198	3.1330	21.9103	1.1278	0.6258	3.1291	13.6092
C9-Zr24	1.1280	0.4314	4.3416	18.8848	1.1278	0.4312	4.3416	18.8848
Zr24-H39	0.4314	0.6808	1.9929	6.7612	0.4312	0.2219	1.6718	5.6741
Zr24-C13	0.4314	1.1359	4.3905	19.0990	0.4312	1.1359	4.3920	19.1044
C13-Zr19	1.1359	0.6269	3.1723	13.7990	1.1359	0.6269	3.1723	13.7990
C13-Zr23	1.2776	0.4209	4.4568	23.2251	1.1359	0.4206	5.7254	19.3918
Zr23-H38	0.4209	0.6796	2.0664	7.0134	0.4206	0.2250	1.5624	5.3027
Zr23-C12	0.4209	1.0254	3.7620	16.3880	0.4206	1.0252	3.7684	16.3907
C12-Zr22	1.0254	0.5658	2.8641	12.4598	1.0252	0.5658	2.1960	12.4543
C12-Zr25	1.0254	0.2866	4.6051	20.0289	1.0252	0.2173	5.0356	21.9022
Zr25-H41	0.2866	0.6656	3.0283	10.2747	0.2173	0.6647	3.5740	12.1290
Zr25-H43	0.2866	0.6438	2.8540	9.6837	0.2173	0.2867	0.2433	1.8814
Zr22-C11	0.5658	1.2776	4.4366	19.2969	0.5658	0.9183	2.1960	9.5563
Zr22-C7	0.5658	1.2273	4.1227	17.9333	0.5658	1.2267	4.1198	17.9170
Zr18-C7	0.5796	1.2273	4.0363	17.5591	0.5794	1.2267	4.0348	17.5483
Zr18-C6	0.5796	0.6358	0.3499	1.5236	0.5794	0.6273	0.2980	1.2986
C6-H33	0.6358	1.2751	8.2036	17.3314	0.6273	0.5017	1.6113	3.4050
C6-Zr17	0.6358	0.4387	1.2283	5.3434	0.6273	0.4163	1.3147	5.7202
Zr17-C11	0.4387	1.2776	5.2286	22.7426	0.4163	0.9183	3.1291	13.6092
C7-Zr19	1.2273	0.6269	3.7425	16.2768	1.2267	0.6269	3.7382	16.2606
Zr19-C8	0.6269	1.2506	3.8880	16.9085	0.6269	1.2506	3.8880	16.9085
Zr14-C8	0.5961	1.2506	7.4232	17.7435	0.5960	1.2506	4.0795	17.7462
Zr14-C2	0.5961	0.7081	0.6969	3.0363	0.5960	0.7078	0.6955	3.0309
C2-H30	0.7081	1.2580	7.0574	14.9078	0.7078	0.4551	3.2428	6.8507
Zr18-C2	0.5796	0.7081	0.8006	3.4836	0.5794	0.7078	0.7992	3.4809

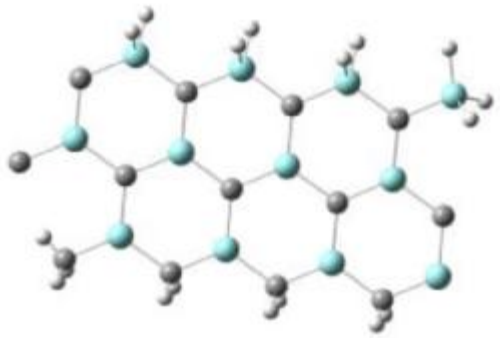

Figure 1. Structure of ZrC nano-sheet.

Table 4. EPR calculated parameters for the ZrC nano-sheet.

atomic bond	V_3 (a.u.)	V_4 (a.u.)	ΔV_{34} (V)	$\Delta V'_{34}$ (V)	V_7 (a.u.)	V_8 (a.u.)	ΔV_{78} (V)	$\Delta V'_{78}$ (V)
C1-H26	862.8161	2.9990	11086.4218	23309.6416	866.8161	3.1666	11084.2704	23413.5379
C1-H27	866.8161	2.9555	11086.9805	23419.2609	866.8161	3.1695	11084.2344	23413.4593
C1-Zr15	866.8161	0.5436	5400.1397	23484.6475	866.8161	0.5447	5400.1324	23484.6177
Zr15-C4	0.5436	871.2802	27.8280	23605.6692	0.5447	871.2802	5427.9604	23605.6394
Zr15-C3	0.5436	867.9012	6.7637	23514.0645	0.5447	867.9012	5406.8976	23514.0347
C3-H31	867.9012	2.8977	11101.6483	23450.2449	867.9012	3.1279	11098.6934	23444.0042
C3-Zr14	867.9012	0.5961	40287.7195	23512.6413	867.9012	0.5961	5406.5764	23512.6413
Zr14-C8	0.5961	871.3152	5970.6446	23605.1948	0.5961	871.3153	21.2817	23605.1975
C8-Zr20	871.3152	0.6258	5427.6739	23604.3896	871.3153	0.6258	5427.6739	23604.3923
Zr20-C4	0.6258	871.2802	5427.4550	23603.4408	0.6258	871.2802	5427.4550	23603.4408
C4-Zr16	871.2802	0.5042	5428.2139	23606.7374	871.2802	0.5077	5428.1908	23606.6425
Zr16-C5	0.5042	876.2953	5459.4763	23742.6967	0.5077	876.2969	5459.4648	23742.6452
Zr16-C10	0.5042	874.0865	5445.7070	23682.8162	0.5077	847.0871	5445.6897	22950.7675
C10-Zr21	874.0865	0.3656	5446.5710	23686.5736	847.0871	0.3677	5446.5624	22954.5629
Zr21-H36	1.4907	2.8202	19.6142	36.0427	0.3677	2.8908	20.1614	68.4012
Zr21-C9	1.4907	871.5558	5430.7958	23587.4649	0.3677	871.5558	5430.7828	23617.9094
C9-Zr20	871.5558	0.6258	5429.1729	23610.9123	871.5558	0.6258	5429.1729	23610.9123
C9-Zr24	871.5558	0.4312	5431.7188	23616.1879	871.5558	0.4315	5430.3840	23616.1798
Zr24-H39	0.4312	2.8207	20.8022	64.7793	1.3723	2.8932	19.6704	41.2316
Zr24-C13	0.4312	871.5556	5430.3854	23616.1825	0.4315	871.5556	5430.3840	23616.1744
C13-Zr19	871.5556	0.6269	5429.1657	23610.8771	871.5556	0.6269	5429.1657	23610.8771
C13-Zr23	871.5556	0.4207	5430.4502	23616.4671	871.5556	0.4209	5430.4488	23616.4617
Zr23-H38	0.4207	2.8219	19.1880	65.0965	0.4209	2.8938	19.7611	67.0403
Zr23-C12	0.4207	871.5611	5430.4848	23616.6162	0.4209	871.5611	5430.4833	23616.6108
C12-Zr22	871.5611	0.5658	5429.5804	23612.6826	871.5611	0.5658	5429.5804	23612.6826
C12-Zr25	871.5611	0.2174	5431.7520	23622.1277	871.5611	0.2866	5431.3214	23620.2517
Zr25-H41	0.2174	2.9038	21.4660	72.8283	0.2866	2.9040	20.9145	70.9577
Zr25-H43	0.2174	2.8434	20.9836	71.1909	0.2866	2.9013	20.8929	70.8845
Zr22-C11	0.5658	873.6436	5442.5620	23669.1392	0.5658	873.6440	5442.5649	23669.1500
Zr22-C7	0.5658	871.3077	5428.0008	23605.8129	0.5658	871.3077	5428.0008	23605.8129
Zr18-C7	0.5794	871.3077	5427.9158	23605.4442	0.5796	871.3077	5427.9144	23605.4388
Zr18-C6	0.5794	867.9066	5406.7147	23513.2404	0.5796	867.9066	5406.7132	23513.2350
C6-H33	867.9066	2.9072	11101.5965	23450.1337	867.9066	3.1347	11098.6762	23443.9662
C6-Zr17	867.9066	0.4163	5407.7313	23517.6620	867.9066	0.4388	5407.5902	23517.0521
Zr17-C11	0.4163	873.6436	5443.4937	23673.1921	0.4388	873.6440	5443.3569	23672.5930
C7-Zr19	871.3077	0.6269	5427.6192	23604.1565	871.3077	0.6269	5427.6192	23604.1565
Zr19-C8	0.6269	871.3152	5427.6667	23604.3598	0.6269	871.3153	5427.6667	23604.3625
Zr14-C8	0.5961	871.3153	5970.6446	23605.1975	0.5961	871.3153	5431.2033	23605.1975
Zr14-C2	0.5961	867.8919	5406.5188	23512.3891	0.5961	867.8919	5406.5188	23512.3891
C2-H30	867.8919	2.8973	11101.5346	23450.0036	867.8919	3.2468	11097.0490	23440.5287
Zr18-C2	0.5794	867.8919	5406.6225	23512.8419	0.5796	867.8919	5406.6211	23512.8365

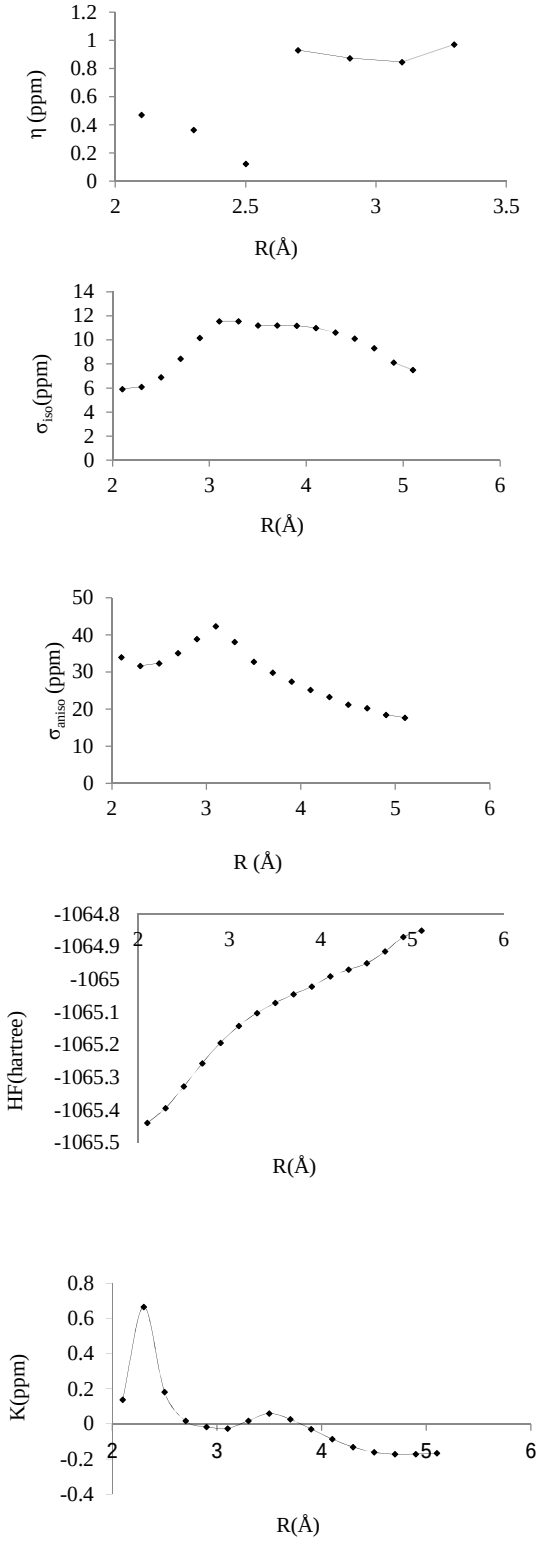

Figure 2. Diagrams of η, σ_{aniso}, σ_{iso}, HF and K of ZrC nano-sheets with different distance (R) of He.

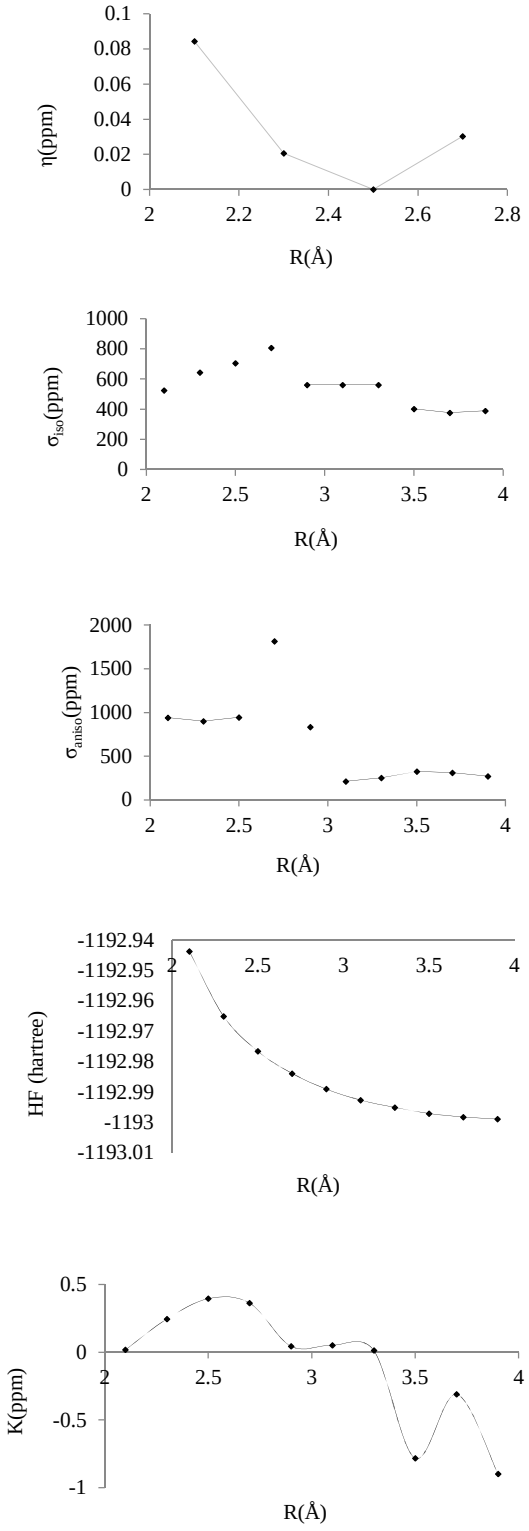

Figure 3. Diagrams of η, σ_{aniso}, σ_{iso}, HF and K of ZrC nano-sheets with different distance (R) of Ne

Table 5. NMR calculated parameters (ppm) for ZrC nano-sheets.

Element	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11
σ_{iso}	141.96	43.16	56.39	-179.19	29136.49	-6.20	-442.05	-1046.76	-1425.72	-21223.15	-403.53
σ_{aniso}	65.40	180.07	160.56	1707.28	124456.00	188.85	779.98	1385.54	5094.02	78717.80	601.11
Ω	105.56	207.48	204.91	1909.02	132544.60	233.63	890.17	2247.63	6016.72	79720.61	846.94
K	-0.52	0.00	0.13	0.57	0.75	0.23	0.50	-0.53	0.39	0.94	-0.16
η		0.46	0.87	0.41		0.79		0.55		0.27	
ξ	43.60	120.04	107.03	1138.18	82971.09	125.90	519.99	923.69	3396.01	52478.53	400.74
R	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
σ_{iso}	153.45	3.88	24.62	-14.04	40918.97	-5.50	-509.65	-430.98	-1043.45	29525.46	-709.89
σ_{aniso}	102.46	142.55	85.92	210.45	164676.10	143.82	464.45	499.71	5622.66	104482.51	1241.93
Ω	178.92	191.69	159.17	2120.08	171737.20	191.02	540.21	726.27	7577.59	106169.90	1565.31
K	-0.71	-0.03	0.02	0.98	0.84	0.01	0.44	-0.25	-0.03	0.94	0.17
η				0.26	0.00			0.34	0.74	0.31	0.07
ξ	68.31	95.03	57.28	1406.30	109784.10	95.88	309.63	333.14	3748.44	69655.01	827.95
R	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10
σ_{iso}	154.57	6.62	25.92	5.64	42357.01	0.36	-490.29	-417.69	-1164.12	30616.87	-703.76
σ_{aniso}	101.78	143.07	83.64	2164.73	169836.30	137.31	464.25	633.11	5771.51	107709.13	1185.63
Ω	183.01	187.17	159.02	2181.16	176587.80	186.86	536.26	804.41	7900.71	109413.57	1503.48
K	-0.78	0.06	-0.90	0.97	0.85	-0.06	0.46	0.15	-0.08	0.94	0.15
η		0.95		0.21				0.34	0.73	0.31	0.04
ξ	67.86	95.38	55.76	1443.15	113224.20	91.54	309.50	422.07	3847.67	71806.09	790.42
R	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50
σ_{iso}	158.23	20.11	37.46	37.43	45630.36	-7.09	-517.82	-466.09	-903.80	32698.15	-687.47
σ_{aniso}	104.51	138.38	99.08	2218.61	181147.00	111.53	234.93	539.41	5431.11	114385.07	1442.14
Ω	188.01	179.31	179.48	2244.48	187815.40	156.62	416.65	788.02	7176.18	116222.32	1675.77
K	-0.78	0.09	-0.79	0.95	0.86	-0.15	-0.74	-0.26	0.03	0.31	0.44
η		0.89		0.20		0.82	0.28	0.80	0.77	0.32	1.00
ξ	69.68	92.25	66.05	1479.07	120764.70	74.36	156.62	359.61	3620.74	76256.71	961.42
R	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70
σ_{iso}	159.08	8.84	25.70	141.39	55597.53	-21.07	-704.10	-359.77	-1938.58	40217.86	-563.20
σ_{aniso}	132.00	117.29	135.06	2693.51	216551.90	60.15	831.45	1173.07	7488.47	137412.19	2091.16
Ω	242.05	138.06	191.27	2762.75	221357.60	100.79	1097.97	1260.22	10938.03	139459.76	2300.61
K	-0.82	0.40	-0.18	0.87	0.91	0.61	0.03	0.72	-0.26	0.00	0.64
η	0.20	0.68	0.87	0.04		0.84	0.83	0.28	0.67	0.31	0.78
ξ	88.00	78.19	90.04	1795.68	144368.00	40.10	0.83	782.05	4992.31	91608.13	1394.11
R	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.30
σ_{iso}	183.40	133.88	151.11	-28.19	33177.84	128.20	-382.42	-673.18	127.77	24859.92	-1650.17
σ_{aniso}	74.46	503.06	529.69	1201.57	140085.90	543.48	1826.70	1421.05	2922.23	88258.42	4137.09
Ω	108.27	537.19	585.71	1461.90	147807.00	572.39	2010.45	1919.16	3450.95	89278.21	5489.37
K	-0.08	0.00	0.62	0.29	0.75	0.12	0.63	0.04	0.39	0.95	0.00
η	0.73	0.21	0.42	0.30		0.20	0.18	0.62	0.89	0.27	0.90
ξ	49.64	335.38	353.13	801.05	0.59	362.32	1217.80	947.37	1948.15	58838.95	2758.06
R	3.90	3.90	3.90	3.90	3.90	3.90	3.90	3.90	3.90	3.90	3.90

Table 6. NMR calculated parameters (ppm) for ZrC nano-sheets.

Element	C12	C13	Zr14	Zr15	Zr16	Zr17	Zr18	Zr19	Zr20	Zr21	Zr22
σ_{iso}	308.78	59.34	-28.87	-511.31	393.36	-120.51	-324.30	-515.69	-546.16	58.46	-331.48
σ_{aniso}	2901.62	4742.28	1127.42	663.61	4229.25	1436.27	589.99	537.79	910.34	1449.06	455.05
Ω	3570.57	6145.63	1199.00	735.60	4598.37	2035.54	793.35	874.17	1060.93	1787.56	661.05
K	0.25	0.09	0.76	0.60	0.67	-0.18	-0.03	-0.54	0.43	0.24	-0.24
η	0.66	0.89	0.20		0.49	0.83			0.78		
ξ	1934.41	3161.52	751.61	442.41	2819.50	957.51	393.33	358.53	606.90	966.04	303.36
R	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
σ_{iso}	-567.40	-175.82	-175.82	-613.57	668.74	-1268.09	-391.66	-826.79	-609.44	111.12	-576.51
σ_{aniso}	842.25	1347.12	1347.12	835.19	5511.09	1589.26	120.54	884.44	939.96	2180.67	460.78
Ω	880.45	1566.61	1566.61	1153.98	5973.55	2298.68	210.19	1365.25	1180.78	2552.61	659.41
K	0.83	0.44	0.44	-0.11	0.69	-0.23	-0.71	-0.41	0.18	0.42	-0.20
η		0.86	0.86	0.92	0.48	0.79	0.39	0.69	0.17		0.86
ξ	561.50	898.08	898.08	556.79	3674.06	1059.50	80.36	589.63	626.64	1453.78	307.19
R	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10
σ_{iso}	-566.39	-21.57	-1074.78	-611.72	716.78	-1257.60	-384.27	-908.02	-605.39	122.93	-568.21
σ_{aniso}	783.53	1890.39	1144.37	828.49	5684.25	1558.85	137.75	983.19	997.36	2260.83	436.15
Ω	846.69	2051.45	1971.40	1148.60	6160.43	2242.83	258.33	1594.83	1257.91	2645.94	615.06
K	0.70	0.75	-0.68	-0.11	0.69	-0.22	-0.87	-0.53	0.17	0.14	-0.05
η		0.55	0.40	0.90	0.47	0.80	0.24	0.57	0.14		0.89
ξ	522.35	1260.26	762.91	552.33	3789.50	1039.23	91.83	655.46	664.91	1507.22	290.76
R	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50
σ_{iso}	-564.08	-626.10	-747.90	-563.28	798.24	-1375.58	-697.80	-482.61	-534.98	149.24	-593.10
σ_{aniso}	1451.67	955.69	687.90	743.03	6031.68	1714.87	543.73	370.98	910.60	2436.15	456.05
Ω	1660.35	1083.02	1037.83	981.81	6543.49	2561.41	834.80	389.14	1066.39	2856.28	668.22
K	0.50	0.53	-0.35	0.03	0.69	-0.32	-0.39	0.81	0.42	0.41	-0.27

η	967.78		0.72	1.00	0.46	0.71	0.61	0.01	0.25		0.80	
ξ	967.78	637.13	458.60	495.35	4021.12	1143.25	362.49	247.32	607.06	1624.10	304.04	
R	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70	
σ_{iso}	-1416.79	1957.03	-1536.25	-647.68	1109.40	-1630.78	-919.82	-1107.18	-583.75	-244.56	-630.17	
σ_{aniso}	2282.04	7407.15	2031.50	971.39	7142.09	2130.79	1025.87	1346.97	1387.11	2980.82	556.33	
Ω	3509.60	7757.94	3584.30	1378.76	7731.92	3373.56	1695.70	2265.78	1762.43	3489.53	844.65	
K	-0.40	0.82	-0.73	-0.18	0.69	-0.47	-0.58	-0.62	0.15	0.42	-0.37	
η	0.63	0.14	0.31	0.80	0.46	0.58	0.38	0.48	0.07		0.75	
ξ	1521.36	4938.10	1354.33	647.59	4761.39	1420.53	683.91	897.98	924.74	1987.21	370.89	
R	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.30	
σ_{iso}	733.65	-3468.06	-3456.39	-141.28	569.83	757.15	2262.89	1540.49	162.78	-11.64	170.01	
σ_{aniso}	9217.60	7098.84	11898.29	1401.13	4820.61	4438.25	8272.27	5900.23	2229.71	1645.47	2137.07	
Ω	9996.39	12412.96	12097.05	1637.65	5134.03	4832.42	8388.26	6057.04	2270.12	1927.42	2257.18	
K	0.69	0.71	0.93	0.42	0.76	0.67	0.94	0.90	0.93	0.41	0.79	
η	0.28	0.02	0.05	0.51	0.50	0.28	0.05	0.08	0.04		0.27	
ξ	6145.07	4732.56	7932.19	934.09	3213.74	2958.83	5514.85	3933.49	1486.47	1096.98	1424.71	
R	3.90	3.90	3.90	3.90	3.90	3.90	3.90	3.90	3.90	3.90	3.90	

The highest and lowest stabilization energy in ZrC nano-sheet were 181.25 and 0.93 kcal/mol for [LP*(2) Zr18, BD*(1) C7-Zr18] and [BD (1) C4-Zr15, RY*(8) Zr20], respectively.

Table 10 shows the bonding and anti-bonding orbitals and hybridization of atomic orbitals in ZrC nano-sheet.

The orbital occupancy is the number of electrons, or "natural population" of the orbital, and the orbital energy is in atomic units: 1 a.u. = 627.5 kcal/mol.

The number of core (CR), 2-center bond (BD) and lone pair (LP) NBOs are in the natural Lewis structure; these labels give the type (BD for 2-center bond, CR for 1-center core pair, LP for 1-center valence lone pair, RY* for 1-center Rydberg, and BD* for 2-center anti-bond) the un-starred and starred labels corresponding to the Lewis and non-Lewis NBOs, respectively.

Table 7. NMR calculated parameters (ppm) for ZrC nano-sheets.

Element	Zr23	Zr24	Zr25	H26	H27	H28	H29	H30	H31	H32	H33
σ_{iso}	-256.11	-381.93	-395.75	160.25	69.74	69.73	30.79	30.80	34.80	34.80	27.55
σ_{aniso}	301.41	112.91	121.69	450.61	106.18	106.20	21.92	21.91	15.46	15.39	39.26
Ω	387.79	441.70	182.54	519.96	126.02	126.04	23.55	23.51	22.54	22.43	60.95
K	0.11	-0.10	-0.33	0.47	-0.42	0.37	0.72	0.73	-0.26	-0.26	-0.42
η	0.79		0.38				0.46	0.46	0.32	0.32	
ξ	200.94	75.28	81.12	300.40	70.79	70.80	14.61	14.61	10.31	10.26	26.18
R	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
σ_{iso}	-305.22	-371.76	-309.43	200.21	80.21	80.61	27.69	28.83	29.46	29.79	23.43
σ_{aniso}	54.93	138.01	60.33	621.78	156.13	156.80	26.61	26.16	31.08	31.82	34.77
Ω	69.67	254.47	98.78	711.72	180.91	181.82	43.03	41.18	46.40	47.53	48.10
K	0.15	-0.83	-0.56	0.16	0.45	0.45	-0.53	-0.46	-0.32	-0.32	-0.11
η	1.00		0.32				0.36	0.32	0.23	0.24	0.51
ξ	36.62	92.00	40.22	414.52	104.09	104.53	17.74	17.44	20.72	21.22	23.18
R	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10
σ_{iso}	-301.52	-374.73	-310.52	205.03	81.85	82.29	27.37	28.24	29.51	30.30	23.88
σ_{aniso}	60.85	146.38	59.77	643.38	163.02	163.63	28.94	26.60	32.26	33.28	34.60
Ω	68.48	265.86	96.70	735.61	188.21	189.19	46.32	43.36	48.20	49.88	47.58
K	0.18	-0.80	-0.53	0.50	0.46	0.46	-0.50	-0.55	-0.32	-0.33	-0.09
η	0.38		0.33				0.24	0.15	0.30	0.31	0.48
ξ	40.56	97.59	39.84	428.92	108.68	109.09	19.29	17.73	21.51	22.19	23.06
R	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50
σ_{iso}	-325.20	-363.81	-305.35	-219.59	85.73	86.16	27.01	28.38	32.11	32.10	22.08
σ_{aniso}	51.56	141.61	52.14	686.10	172.25	173.63	31.23	22.70	30.48	27.32	38.55
Ω	95.38	268.93	102.14	779.00	197.31	198.71	34.32	27.20	42.12	39.48	50.79
K	-0.84	-0.89	-0.96	0.52	0.49	0.50	0.64	0.34	-0.10	-0.23	0.04
η	0.20	94.41	0.04				0.66	0.67	0.49	0.36	0.59
ξ	34.38	94.41	34.76	457.40	114.83	115.76	20.82	15.13	20.32	18.22	25.70
R	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70
σ_{iso}	-308.86	-369.81	-300.88	250.24	95.45	96.15	24.41	24.06	31.18	30.53	14.44
σ_{aniso}	73.12	200.70	151.98	838.44	219.40	220.75	31.60	30.91	52.99	51.35	49.86
Ω	92.25	358.46	241.55	951.07	249.60	250.98	51.37	51.16	78.52	77.00	64.74
K	0.01	-0.76	-0.48	0.53	0.52	0.52	0.54	-0.58	-0.30	-0.33	0.08
η	0.75		0.23				0.34	0.25	0.60	0.56	
ξ	48.74	133.80	101.32	558.96	146.27	147.17	21.07	20.61	35.32	34.23	33.24
R	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.30
σ_{iso}	-381.54	-292.79	-379.97	196.89	87.49	86.74	47.01	44.10	65.02	65.73	67.37
σ_{aniso}	177.07	358.92	550.47	485.77	127.46	124.12	56.47	56.44	167.62	169.38	129.52
Ω	246.00	510.61	891.29	534.86	140.63	136.44	73.04	76.00	204.97	207.17	153.76
K	-0.12	-0.19	-0.53	0.63	0.63	0.64	0.09	-0.03	0.27	0.27	0.37
η	0.38		0.84						0.01	0.07	
ξ	118.04	239.28	336.98	323.85	84.97	82.75	37.65	37.63	111.75	112.92	86.35
R	3.90	3.90	3.90	3.90	3.90	3.90	3.90	3.90	3.90	3.90	3.90

Tables 11-15 allow quick identification of the principal delocalizing acceptor orbitals associated with each donor NBO, and their topological relationship with NBO, that is, whether they are attached to the same atom (geminal, "g"), or to an adjacent bonded atom (vicinal, "v"), or to a more remote ("r") site. For example, from Tables 11-15, the highest-occupancy, highest-energy and primarily delocalized were 1.99986 electrons, -10.0997 a.u. and 137(v) for CR (1) C5, respectively. ,However, the lowest-occupancy, was 0.00002 electrons for RY*(9) Zr15.

Table 8. NMR calculated parameters (ppm) for ZrC nano-sheets.

Element	H34	H35	H36	H37	H38	H39	H40	H41	H42	H43	He44	Ne44
σ_{iso}	27.56	101.04	101.04	29.42	29.42	34.23	34.23	24.53	20.15	20.15	0.00	27.56
σ_{aniso}	39.24	239.51	239.49	15.62	15.50	46.00	45.95	15.52	23.89	23.89	0.00	39.24
Ω	60.91	252.79	252.76	20.39	20.25	59.35	59.30	25.35	41.44	41.40	0.00	60.91
K	-0.42	0.79	0.79	0.06	0.06	0.10	0.10	-0.55	-0.69	-0.69	0.00	-0.42
η				0.18	0.18	0.12	0.12		0.71	0.71	0.00	
ξ	26.16	159.68	159.66	10.41	10.34	30.66	30.63	10.35	15.93	15.93	0.00	26.16
R	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
σ_{iso}	24.41	123.98	124.04	29.07	30.33	39.62	38.93	24.78	24.04	24.34	5.91	24.41
σ_{aniso}	33.85	326.61	326.52	27.71	29.83	55.02	49.69	12.21	18.81	18.11	33.94	33.85
Ω	48.95	343.18	342.98	36.21	37.93	64.91	60.84	20.68	32.39	31.76	39.77	48.95
K	-0.23	0.81	0.81	0.06	0.05	0.13	0.27	-0.64	-0.68	-0.72	0.14	-0.23
η	0.52			0.24	0.34	0.17	0.22				0.47	0.52
ξ	22.56	217.74	217.68	18.47	19.89	36.68	33.12	8.14	12.54	12.07	22.63	22.56
R	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10	2.10
σ_{iso}	24.94	126.72	127.08	29.43	30.90	40.15	39.53	24.83	24.14	24.41	6.90	24.94
σ_{aniso}	33.79	337.13	337.76	27.59	30.70	56.78	50.19	12.26	18.88	18.16	32.35	33.79
Ω	48.78	354.50	354.93	36.20	38.80	66.44	61.73	20.68	32.61	31.95	40.67	48.78
K	-0.23	0.80	0.81	0.05	0.16	0.42	0.25	-0.63	-0.68	-0.72	0.18	-0.23
η	0.50			0.24	0.40	0.14	0.22		12.59		0.12	0.50
ξ	22.53	224.75	225.18	18.39	20.46	37.85	33.46	8.18	12.59	12.10	21.57	22.53
R	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50
σ_{iso}	23.60	133.99	133.38	30.11	28.86	41.43	41.03	25.70	24.59	24.41	11.20	0.00
σ_{aniso}	39.67	356.58	355.88	31.39	27.30	60.49	56.46	10.63	17.95	17.99	29.87	0.00
Ω	51.71	373.39	372.76	39.77	36.36	69.42	66.52	19.40	31.78	30.89	39.47	0.00
K	0.07	0.82	0.82	0.16	0.00	0.49	0.40	-0.81	-0.74	-0.67	0.03	0.00
η	0.65			0.25	0.13	0.33	0.35					0.00
ξ	26.45	237.72	237.25	20.93	18.20	40.33	37.64	7.09	11.97	11.99	19.91	0.00
R	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70	3.70	0.00
σ_{iso}	16.56	155.53	154.42	32.85	31.31	47.11	46.97	28.29	23.46	24.05	0.00	643.11
σ_{aniso}	49.55	438.77	435.51	34.86	43.34	60.04	60.18	12.88	22.52	21.46	0.00	898.70
Ω	64.06	461.39	458.31	48.94	57.49	68.19	69.42	21.62	37.13	36.05	0.00	1107.73
K	0.09	0.80	0.27	0.15	0.02	0.52	0.47	-0.62	-0.57	-0.62	0.00	0.25
η	0.95			0.15	0.03	0.30	0.31				0.00	0.02
ξ	33.03	292.51	290.34	23.24	28.90	40.03	40.12	8.59	15.01	14.30	0.00	599.13
R	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.30	0.00	2.30
σ_{iso}	65.62	109.09	110.97	19.39	24.88	30.23	34.19	16.09	33.33	33.30	0.00	-388.79
σ_{aniso}	133.60	255.72	260.18	37.72	37.65	53.68	49.51	48.64	40.06	43.65	0.00	270.40
Ω	159.30	268.32	272.67	51.23	48.48	69.85	69.78	81.22	52.08	56.50	0.00	514.57
K	0.35	0.81	0.27	0.06	0.11	0.07	0.06	-0.60	0.08	0.17	0.00	-0.90
η				0.35	0.67	0.66	0.95	0.30	0.31	0.45	0.00	0.05
ξ	89.07	170.48	173.45	25.15	25.10	35.79	33.01	32.42	26.71	29.10	0.00	180.26
R	3.90	3.90	3.90	3.90	3.90	3.90	3.90	3.90	3.90	3.90	0.00	3.90

Table 9. Donor NBO, acceptor NBO, E2, Ei- Ej and F(i,j) for ZrC nano-sheet.

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(i)-E(j) a.u.	F (i , j) a.u.
BD(1) C1-Zr15	LP*(2) Zr15	1.02	0.54	0.02
BD(1) C1-Zr15	LP*(2) Zr16	1.29	0.59	0.03
BD(1) C1-Zr15	RY*(5) Zr15	2.08	1.80	0.06
BD(1) C4-Zr15	RY*(8) Zr20	0.93	1.55	0.03
BD(1) C4-Zr16	LP*(3) Zr15	8.10	0.58	0.06
BD(1) C4-Zr16	RY*(2) Zr15	1.61	0.77	0.03
BD(1) C4-Zr16	BD*(1) C4-Zr15	1.96	0.51	0.03
BD(1) C7-Zr22	LP*(4) Zr15	8.09	0.48	0.06
BD(1) C7-Zr22	LP*(1) Zr19	42.10	0.58	0.15
BD(1) C7-Zr22	RY*(6) Zr20	4.81	3.70	0.13
BD(1) C8-Zr14	LP*(4) Zr20	17.58	0.60	0.09
BD(1) C8-Zr14	RY*(5) Zr14	4.79	2.04	0.09
BD(1) C8-Zr14	BD*(1) C2-Zr14	4.31	0.64	0.05
BD(3) C11-Zr17	LP*(1) Zr22	20.44	0.28	0.07
BD(3) C11-Zr17	RY*(1) C6	15.78	2.21	0.18
BD(3) C11-Zr17	BD*(2) C7-Zr18	5.40	0.21	0.03
CR(1) Zr14	LP*(4) Zr14	2.96	2.00	0.07
CR(1) Zr14	RY*(2) C3	1.31	4.47	0.07
CR(3) Zr14	BD*(1) C8-Zr14	8.12	1.41	0.10
CR(3) Zr24	BD*(1) C9-Zr24	2.06	1.42	0.05
CR(1) Zr25	LP* Zr23	1.28	2.13	0.05
CR(1) Zr25	RY*(1) C12	1.38	4.31	0.07
CR(3) Zr25	BD*(1) Zr25-H41	7.11	1.48	0.09
LP(1) C4	LP*(3) Zr16	65.91	0.06	0.07
LP(1) C4	RY*(3) C4	2.59	0.65	0.05
LP(1) C4	BD*(2) C9-Zr20	3.51	0.12	0.02
LP(1) C10	RY*(6) Zr21	1.56	2.23	0.06
LP(2) C10	LP*(1) Zr21	17.10	0.22	0.07
LP(2) C10	BD*(1) C10-Zr16	8.62	0.23	0.05
LP*(3) C10	LP*(3) Zr16	9.49	0.03	0.02
LP*(3) C10	RY*(3) Zr16	4.56	0.12	0.04
LP(1) C11	LP*(1) Zr22	73.50	0.62	0.20
LP*(2) Zr16	LP*(5) Zr16	36.02	0.08	0.13
LP*(2) Zr16	RY*(1) C4	9.82	2.44	0.40
LP*(2) Zr16	BD*(1) C9-Zr21	2.65	0.02	0.02
LP*(2) Zr18	BD*(1) C7-Zr18	181.25	0.02	0.19
LP*(1) Zr19	LP*(6) Zr21	1.45	0.03	0.01
BD*(1) C4-Zr16	LP*(2) Zr15	3.91	0.03	0.02
BD*(1) C4-Zr16	RY*(5) Zr16	6.47	0.86	0.19
BD*(1) C4-Zr16	BD*(1) C4-Zr16	26.24	0.06	0.09
BD*(1) C4-Zr20	LP*(3) Zr20	25.68	0.04	0.08
BD*(1) C4-Zr20	RY*(2) C9	2.46	2.04	0.26
BD*(1) C4-Zr20	BD*(1) C9-Zr21	3.06	0.04	0.04
BD*(1) C7-Zr22	LP*(6) Zr22	32.44	0.07	0.14
BD*(1) C7-Zr22	RY*92) C11	2.49	1.06	0.16
BD*(1) C7-Zr22	BD*(1) C6-Zr18	8.49	0.02	0.04
BD*(2) C8-Zr14	LP*(1) Zr20	19.48	0.06	0.06
BD*(2) C8-Zr14	RY*(8) Zr14	1.77	1.25	0.14
BD*(2) C8-Zr14	BD*(1) C2-Zr14	6.81	0.23	0.10
BD*(1) C10-Zr16	LP*(5) Zr16	18.85	0.17	0.14
BD*(1) C10-Zr16	RY*(1) C4	6.46	2.54	0.32
BD*(1) C10-Zr16	BD*(1) C4-Zr20	9.96	0.07	0.06

Table 10. NBO data obtained for ZrC nano-sheet.

Bond orbital	Coefficient/Hybrids	Anti-bond orbital c	Coefficient/Hybrids
BD(1) C1-Zr15	$0.8776*(sp^{3.23})C + 0.4795*(sp^{0.21}d^{3.93})Zr$	BD*(1) C1-Zr15	$0.4795*(sp^{3.23})C - 0.8776*(sp^{0.21}d^{3.93})Zr$
BD(1) C1-H26	$0.7918*(sp^{2.88})C + 0.6108*(s)H$	BD*(1) C1-H26	$0.6108*(sp^{2.88})C - 0.7918*(s)H$
BD(1) C1-H27	$0.7828*(sp^{2.98})C + 0.6223*(s)H$	BD*(1) C1-H27	$0.6223*(sp^{2.98})C - 0.7828*(s)H$
BD(1) C1-H28	$0.7828*(sp^{2.98})C + 0.6223*(s)H$	BD*(1) C1-H28	$0.6223*(sp^{2.98})C - 0.7828*(s)H$
BD(1) C2-Zr14	$0.9037*(sp^{2.69})C + 0.4281*(sp^{1.12}d^{2.32})Zr$	BD*(1) C2-Zr14	$0.4281*(sp^{2.69})C - 0.9037*(sp^{1.12}d^{2.32})Zr$
BD(1) C2-Zr18	$0.9048*(sp^{2.61})C + 0.4258*(sp^{0.97}d^{2.11})Zr$	BD*(1) C2-Zr18	$0.4258*(sp^{2.61})C - 0.9048*(sp^{0.97}d^{2.11})Zr$
BD(1) C2-H29	$0.7880*(sp^{3.45})C + 0.6157*(s)H$	BD*(1) C2-H29	$0.6157*(sp^{3.45})C - 0.7880*(s)H$
BD(1) C2-H30	$0.7880*(sp^{3.45})C + 0.6157*(s)H$	BD*(1) C2-H30	$0.6157*(sp^{3.45})C - 0.7880*(s)H$
BD(1) C3-Zr14	$0.9012*(sp^{2.66})C + 0.4333*(sp^{1.63}d^{4.50})Zr$	BD*(1) C3-Zr14	$0.4333*(sp^{2.66})C - 0.9012*(sp^{1.63}d^{4.50})Zr$
BD(1) C3-Zr15	$0.8908*(sp^{2.71})C + 0.4544*(sp^{0.32}d^{4.53})Zr$	BD*(1) C3-Zr15	$0.4544*(sp^{2.71})C - 0.8908*(sp^{0.32}d^{4.53})Zr$
BD(1) C3-H31	$0.7881*(sp^{3.40})C + 0.6155*(s)H$	BD*(1) C3-H31	$0.6155*(sp^{3.40})C - 0.7881*(s)H$
BD(1) C3-H32	$0.7881*(sp^{3.40})C + 0.6155*(s)H$	BD*(1) C3-H32	$0.6155*(sp^{3.40})C - 0.7881*(s)H$
BD(1) C4-Zr15	$0.8712*(sp^{2.42})C + 0.49098*(sp^{0.46}d^{5.17})Zr$	BD*(1) C4-Zr15	$0.4909*(sp^{2.42})C - 0.8712*(sp^{0.46}d^{5.17})Zr$
BD(1) C4-Zr16	$0.8858*(sp^{2.13})C + 0.4641*(sp^{0.73}d^{8.92})Zr$	BD*(1) C4-Zr16	$0.4641*(sp^{2.13})C - 0.8858*(sp^{0.73}d^{8.92})Zr$
BD(1) C4-Zr20	$0.8942*(sp^{1.57})C + 0.4476*(sp^{0.54}d^{5.04})Zr$	BD*(1) C4-Zr20	$0.4476*(sp^{1.57})C - 0.8942*(sp^{0.54}d^{5.04})Zr$
BD(1) C5-Zr16	$0.8746*(sp^{3.80})C + 0.4848*(sp^{0.25}d^{3.24})Zr$	BD*(1) C5-Zr16	$0.4848*(sp^{3.80})C - 0.8746*(sp^{0.25}d^{3.24})Zr$
BD(1) C6-Zr17	$0.8862*(sp^{3.11})C + 0.4634*(sp^{0.16}d^{2.16})Zr$	BD*(1) C6-Zr17	$0.4634*(sp^{3.11})C - 0.8862*(sp^{0.16}d^{2.16})Zr$
BD(1) C6-Zr18	$0.9026*(sp^{2.68})C + 0.4305*(sp^{1.89}d^{6.20})Zr$	BD*(1) C6-Zr18	$0.4305*(sp^{2.68})C - 0.9026*(sp^{1.89}d^{6.20})Zr$
BD(1) C6-H33	$0.7867*(sp^{3.14})C + 0.6174*(s)H$	BD*(1) C6-H33	$0.6174*(sp^{3.14})C - 0.7867*(s)H$
BD(1) C6-H34	$0.7867*(sp^{3.14})C + 0.6174*(s)H$	BD*(1) C6-H34	$0.6174*(sp^{3.14})C - 0.7867*(s)H$
BD(1) C7-Zr18	$0.8712*(sp^{2.27})C + 0.4909*(sp^{0.45}d^{5.66})Zr$	BD*(1) C7-Zr18	$0.4909*(sp^{2.27})C - 0.8712*(sp^{0.45}d^{5.66})Zr$
BD(2) C7-Zr18	$0.9472*(sp^{12.84})C + 0.3207*(sp^{14.70}d^{13.82})Zr$	BD*(2) C7-Zr18	$0.3207*(sp^{12.84})C - 0.9472*(sp^{14.70}d^{13.82})Zr$
BD(1) C7-Zr22	$0.9044*(sp^{0.61})C + 0.4267*(sp^{0.63}d^{7.05})Zr$	BD*(1) C7-Zr22	$0.4267*(sp^{0.61})C - 0.9044*(sp^{0.63}d^{7.05})Zr$
BD(1) C8-Zr14	$0.8740*(sp^{2.10})C + 0.4860*(sp^{0.4}d^{4.72})Zr$	BD*(1) C8-Zr14	$0.4860*(sp^{2.10})C - 0.8740*(sp^{0.4}d^{4.72})Zr$
BD(2) C8-Zr14	$0.9471*(sp^{25.01})C + 0.3210*(sp^{30.78}d^{28.21})Zr$	BD*(2) C8-Zr14	$0.3210*(sp^{25.01})C - 0.9471*(sp^{30.78}d^{28.21})Zr$
BD(1) C8-Zr19	$0.9085*(sp^{0.57})C + 0.4179*(sp^{0.59}d^{5.89})Zr$	BD*(1) C8-Zr19	$0.4179*(sp^{0.57})C + 0.9085*(sp^{0.59}d^{5.89})Zr$
BD(1) C9-Zr20	$0.8753*(sp^{2.09})C + 0.4837*(sp^{0.32}d^{5.13})Zr$	BD*(1) C9-Zr20	$0.4837*(sp^{2.09})C - 0.4853*(sp^{0.32}d^{5.13})Zr$
BD(2) C9-Zr20	$0.8039*(p^{1})C + 0.5948*(p^{1}d^{21.80})Zr$	BD*(2) C9-Zr20	$0.5948*(p^{1})C - 0.8039*(p^{1}d^{21.80})Zr$
BD(1) C9-Zr21	$0.8813*(sp^{2.13})C + 0.4726*(sp^{0.45}d^{4.07})Zr$	BD*(1) C9-Zr21	$0.4726*(sp^{2.13})C - 0.8813*(sp^{0.45}d^{4.07})Zr$

BD(1) C9-Zr24	$0.8916*(sp^{1.80})C + 0.4528*(sp^{0.45}d^{3.67})Zr$	BD*(1) C9-Zr24	$0.4528*(sp^{1.80})C - 0.8916*(sp^{0.45}d^{3.67})Zr$
BD(1) C10-Zr16	$0.8983*(sp^{99.99})C + 0.4394*(sp^{0.18}d^{3.71})Zr$	BD*(1) C10-Zr16	$0.4394*(sp^{99.99})C - 0.8916*(sp^{0.18}d^{3.71})Zr$
BD(1) C11-Zr17	$0.8766*(sp^{99.99})C + 0.4812*(sp^{0.18}d^{4.28})Zr$	BD*(1) C11-Zr17	$0.4812*(sp^{99.99})C - 0.8766*(sp^{0.18}d^{4.28})Zr$
BD(2) C11-Zr17	$0.7312*(p^{1})C + 0.6822*(p^{1}d^{57.47})Zr$	BD*(2) C11-Zr17	$0.6822*(p^{1})C - 0.7312*(p^{1}d^{57.47})Zr$
BD(3) C11-Zr17	$0.7056*(sp^{99.99})C + 0.7086*(sp^{0.09}d^{2.11})Zr$	BD*(3) C11-Zr17	$0.7086*(sp^{99.99})C - 0.7056*(sp^{0.09}d^{2.11})Zr$
BD(1) C12-Zr22	$0.8775*(sp^{2.03})C + 0.4795*(sp^{0.34}d^{5.15})Zr$	BD*(1) C12-Zr22	$0.4795*(sp^{2.03})C - 0.8775*(sp^{0.34}d^{5.15})Zr$
BD(2) C12-Zr22	$0.8063*(p^{1})C + 0.5919*(p^{1}d^{22.26})Zr$	BD*(2) C12-Zr22	$0.5915*(p^{1})C - 0.8063*(p^{1}d^{22.26})Zr$
BD(1) C12-Zr23	$0.8916*(sp^{1.18})C + 0.4529*(sp^{0.44}d^{3.62})Zr$	BD*(1) C12-Zr23	$0.4529*(sp^{1.18})C - 0.8916*(sp^{0.44}d^{3.62})Zr$
BD(1) C12-Zr25	$0.8824*(sp^{2.18})C + 0.4704 *(sp^{0.32}d^{3.35})Zr$	BD*(1) C12-Zr25	$0.4704*(sp^{2.18})C - 0.8824 *(sp^{0.32}d^{3.35})Zr$
BD(1) C13-Zr19	$0.8788*(sp^{2.12})C + 0.4772*(sp^{0.47}d^{6.50})Zr$	BD*(1) C13-Zr19	$0.4772*(sp^{2.12})C - 0.8788*(sp^{0.47}d^{6.50})Zr$
BD(2) C13-Zr19	$0.7954*(p^{1})C + 0.6061*(p^{1}d^{21.16})Zr$	BD*(2) C13-Zr19	$0.6061*(p^{1})C - 0.7954*(p^{1}d^{21.16})Zr$
BD(1) C13-Zr23	$0.8895*(sp^{1.93})C + 0.4570*(sp^{0.47}d^{3.73})Zr$	BD*(1) C13-Zr23	$0.4570*(sp^{1.93})C - 0.8895*(sp^{0.47}d^{3.73})Zr$
BD(1) C13-Zr24	$0.8895*(sp^{1.96})C + 0.4570*(sp^{0.43}d^{3.66})Zr$	BD*(1) C13-Zr24	$0.4570*(sp^{1.96})C - 0.8895*(sp^{0.43}d^{3.66})Zr$
BD(1) Zr21-H35	$0.6045*(sp^{0.26}d^{2.32})Zr + 0.7966*(s)H$	BD*(1) Zr21-H35	$0.7966*(sp^{0.26}d^{2.32})Zr - 0.6045*(s)H$
BD(1) Zr21-H36	$0.6045*(sp^{0.26}d^{2.32})Zr + 0.7966*(s)H$	BD*(1) Zr21-H36	$0.7966*(sp^{0.26}d^{2.32})Zr - 0.6045*(s)H$
BD(1) Zr23-H37	$0.6024*(sp^{0.25}d^{2.09})Zr + 0.7966*(s)H$	BD*(1) Zr23-H37	$0.7982*(sp^{0.25}d^{2.09})Zr - 0.6024*(s)H$
BD(1) Zr23-H38	$0.6024*(sp^{0.25}d^{2.09})Zr + 0.7982*(s)H$	BD*(1) Zr23-H38	$0.7982*(sp^{0.25}d^{2.09})Zr - 0.6024*(s)H$
BD(1) Zr24-H39	$0.6026*(sp^{0.25}d^{2.10})Zr + 0.7980*(s)H$	BD*(1) Zr24-H39	$0.7980*(sp^{0.25}d^{2.10})Zr - 0.6026*(s)H$
BD(1) Zr24-H40	$0.6026*(sp^{0.25}d^{2.10})Zr + 0.7980*(s)H$	BD*(1) Zr24-H40	$0.7980*(sp^{0.25}d^{2.10})Zr - 0.6026*(s)H$
BD(1) Zr25-H41	$0.5908*(sp^{0.27}d^{2.51})Zr + 0.8068*(s)H$	BD*(1) Zr25-H41	$0.8068*(sp^{0.27}d^{2.51})Zr - 0.5908*(s)H$
BD(1) Zr25-H42	$0.5859*(sp^{0.33}d^{2.54})Zr + 0.8104*(s)H$	BD*(1) Zr25-H42	$0.8104*(sp^{0.33}d^{2.54})Zr - 0.5859*(s)H$
BD(1) Zr25-H43	$0.5860*(sp^{0.33}d^{2.53})Zr + 0.8103*(s)H$	BD*(1) Zr25-H43	$0.8103*(sp^{0.33}d^{2.53})Zr - 0.5860*(s)H$

Table 11. NBO data obtained for ZrC nano-sheet.

Bond orbital	Occupancy	Energy (a.u.)	Principal Delocalizations (geminal,vicinal,remote)
BD(1) C1-Zr15	1.98373	-0.38248	198(v),202(v),379(g),367(g),254(g),376(g),135(r),380(v)
BD(1) C1-H26	1.97552	-0.50224	129(v),376(v),198(r),130(v),
BD(1) C1-H27	1.96990	-0.51236	131(v),129(v),133(v),128(v),250(v),132(v)
BD(1) C1-H28	1.96990	-0.51236	131(v),129(v),133(v),128(v),250(v),132(v)
BD(1) C2-Zr14	1.87635	-0.39438	391(g),388(v),372(g),194(g),390(g),152(r),371(g),217(v)
BD(1) C2-Zr18	1.87918	-0.39632	388(g),391(v),153(r),371(g),194(g),387(g),281(g),372(g)
BD(1) C2-H29	1.94058	-0.52581	125(v),147(v),371(g),372(g),149(v),123(v),145(v),127(v)
BD(1) C2-H30	1.94058	-0.52581	125(v),147(v),371(g),372(g),149(v),123(v),145(v),127(v)
BD(1) C3-Zr14	1.88956	-0.40019	129(v),391(g),159(r),367(v),390(g),250(v),198(g),379(v)
BD(1) C3-Zr15	1.92367	-0.40181	391(v),375(g),198(g),379(g),254(g),202(v),158(r),124(v)
BD(1) C3-H31	1.94199	-0.52777	125(v),131(v),129(v),126(v),375(g),123(v),130(v),128(v)
BD(1) C3-H32	1.94199	-0.52777	125(v),131(v),129(v),126(v),375(g),123(v),130(v),128(v)
BD(1) C4-Zr15	1.84134	-0.37546	158(v),135(v),202(g),367(g),376(g),379(g),254(g),397(v
BD(1) C4-Zr16	1.80468	-0.37983	130(v),156(v),158(v),201(g),376(v),380(g),251(v),266(g)
BD(1) C4-Zr20	1.83764	-0.40757	130(v),135(v),129(v),367(v),202(g),251(v),393(g),300(g)
BD(1) C5-Zr16	1.97472	-0.37614	137(g),397(g),226(v),380(g),201(v),263(g),225(v),130(r)
BD(1) C6-Zr17	1.91668	-0.38631	146(v),384(g),388(v),209(g),229(v),171(r),170(r),276(g)
BD(1) C6-Zr18	1.90495	-0.40200	388(g),170(r),140(v),398(v),143(v),387(g),389(v),209(g)
BD(1) C6-H33	1.94949	-0.53273	141(v),147(v),148(v),143(v),384(g),398(v),145(v),149(v)
BD(1) C6-H34	1.94949	-0.53272	141(v),147(v),148(v),143(v),384(g),398(v),145(v),149(v)
BD(1) C7-Zr18	1.84433	-0.37698	153(r),150(r),170(v),213(g),281(g),283(g),387(g),372(g)
BD(2) C7-Zr18	1.57708	-0.23816	150(r),153(r),372(g),389(g),155(r),401(v),291(r),214(g)
BD(1) C7-Zr22	1.78537	-0.4575	150(r),153(r),152(r),148(v),146(v),318(g),401(g),214(g)
BD(1) C8-Zr14	1.83807	-0.38263	159(r),156(r),152(v),217(g),245(g),390(g),371(g),375(g)
BD(2) C8-Zr14	1.58330	-0.23222	156(r),392(g),371(g),159(r),300(r),375(g),405(v),218(g)
BD(1) C8-Zr19	1.77726	-0.46424	156(r),158(r),159(r),124(v),126(v),405(g),291(g),218(g)
BD(1) C9-Zr20	1.80968	-0.35059	164(v),180(v),222(g),300(g),381(g),393(g),167(v),202(v)
BD(2) C9-Zr20	1.62616	-0.16274	163(v),179(v),113(v),118(r),394(g),182(v),166(v),409(v)
BD(1) C9-Zr21	1.80205	-0.34607	159(v),181(v),221(g),156(v),309(g),310(g),225(r),311(g)
BD(1) C9-Zr24	1.78070	-0.35801	158(v),165(v),159(v),335(g),221(g),162(v),153(r),333(g)
BD(1) C10-Zr16	1.74407	-0.21505	162(r),120(g),309(r),382(g),395(r),310(r),264(g),221(r)
BD(1) C11-Zr17	1.82339	-0.26782	168(r),170(r),389(r),318(r),384(v),210(v),281(r),315(r)
BD(2) C11-Zr17	1.73945	-0.20625	169(r),172(r),402(r),399(g),147(r)
BD(3) C11-Zr17	1.64828	-0.17603	383(g),168(r),209(v),229(g),170(r),276(g),144(g),273(g)
BD(1) C12-Zr22	1.81307	-0.35038	175(v),186(v),185(v),234(g),318(g),152(r),389(g),401(g)
BD(2) C12-Zr22	1.67215	-0.16192	184(v),174(v),117(v),177(v), 402(g),417(v),416(v),411(v)
BD(1) C12-Zr23	1.78745	-0.35910	170(v),186(v),168(v),171(v),185(v),327(g),152(r),233(g)
BD(1) C12-Zr25	1.77135	-0.34288	170(v),176(v),233(g),347(g),345(g),403(g),404(g),407(v)
BD(1) C13-Zr19	1.79781	-0.34458	180(v),175(v),291(g),239(g), 158(r),176(v),181(v),392(g)
BD(2) C13-Zr19	1.66267	-0.15947	179(v),174(v),118(v),117(r),177(v),406(g),182(v),413(v)
BD(1) C13-Zr23	1.77337	-0.34846	152(v),181(v),328(g),237(g),327(g),153(v),325(g),407(g)
BD(1) C13-Zr24	1.78062	-0.3465	153(v),176(v),150(v),237(g),335(g),333(g),338(g),158(r)
BD(1) Zr21-H35	1.97856	-0.27784	181(r),395(g),309(g),221(v),226(r),410(g),311(g),409(g)
BD(1) Zr21-H36	1.97856	-0.27784	181(r),395(g),309(g),221(v),226(r),410(g),311(g),409(g)
BD(1) Zr23-H37	1.97325	-0.26400	407(g),403(g),327(g),412(g), 328(g),181(r),411(g),325(g)
BD(1) Zr23-H38	1.97325	-0.26399	407(g),403(g),327(g),411(g),328(g),181(r),412(g),325(g)
BD(1) Zr24-H39	1.97263	-0.26403	335(g),408(g),396(g),414(g),333(g),176(r),413(g),338(g)
BD(1) Zr24-H40	1.97263	-0.26403	335(g),408(g),396(g),413(g),333(g),176(r),414(g),338(g)
BD(1) Zr25-H41	1.98279	-0.28534	176(r),233(v),403(v),347(g),345(g),415(g),404(g),186(g)
BD(1) Zr25-H42	1.98706	-0.28989	170(r),233(v),401(v),347(g),345(g),416(g),404(g),186(g)
BD(1) Zr25-H43	1.98708	-0.28988	170(r),233(v),401(v),347(g),345(g),417(g),404(g),186(g)

Table 12. NBO data obtained for ZrC nano-sheet.

Anti-bond orbital	occupancy	Energy (a.u.)	Principal Delocalizations (geminal,vicinal,remote)
BD*(1) C1-Zr15	0.08550	0.18061	
BD*(1) C1-H26	0.00541	0.43210	
BD*(1) C1-H27	0.00266	0.41015	
BD*(1) C1-H28	0.00266	0.41015	
BD*(1) C2-Zr14	0.05123	0.26086	
BD*(1) C2-Zr18	0.05282	0.24344	
BD*(1) C2-H29	0.00645	0.38445	
BD*(1) C2-H30	0.00645	0.38445	
BD*(1) C3-Zr14	0.04920	0.20248	
BD*(1) C3-Zr15	0.09122	0.16266	
BD*(1) C3-H31	0.00552	0.38286	
BD*(1) C3-H32	0.00552	0.38286	
BD*(1) C4-Zr15	0.06137	0.14929	
BD*(1) C4-Zr16	0.25867	0.12714	397(g),135(g),382(g),138(g),367(v),263(g),264(g),167(r)
BD*(1) C4-Zr20	0.11472	0.17910	161(g),393(g),367(v),156(g),376(v),158(g),130(v),135(v)
BD*(1) C5-Zr16	0.07495	0.18628	
BD*(1) C6-Zr17	0.05019	0.10942	
BD*(1) C6-Zr18	0.04822	0.16615	
BD*(1) C6-H33	0.00811	0.38476	
BD*(1) C6-H34	0.00811	0.38476	
BD*(1) C7-Zr18	0.07858	0.13874	
BD*(2) C7-Zr18	0.18505	0.03638	391(r),398(r),148(g),372(g),142(r),387(g),389(g),194(v)
BD*(1) C7-Zr22	0.17446	0.14381	178(r),168(g),171(g),173(g),401(g),146(v),387(g),170(g)
BD*(1) C8-Zr14	0.07353	0.16132	
BD*(2) C8-Zr14	0.18042	0.03385	388(r),156(r),371(g),248(g),148(r),126(g),132(r),398(r)
BD*(1) C8-Zr19	0.16937	0.16125	390(g),155(g),150(g),183(r),405(g),152(g),124(v),171(r)
BD*(1) C9-Zr20	0.10944	0.18614	161(g),381(g),158(g),159(g),156(g),152(r),382(r),392(r)
BD*(2) C9-Zr20	0.05482	-0.01496	
BD*(1) C9-Zr21	0.05594	0.22193	
BD*(1) C9-Zr24	0.05313	0.25934	
BD*(1) C10-Zr16	0.24848	0.10963	162(r),380(g),382(g),138(g),137(g),263(g),165(r),381(v)
BD*(1) C11-Zr17	0.10723	0.03839	142(g),388(r),140(g),383(g),168(r),148(r),171(r),274(g)
BD*(2) C11-Zr17	0.01233	-0.06254	
BD*(3) C11-Zr17	0.07111	-0.04834	
BD*(1) C12-Zr22	0.11810	0.18386	173(g),170(g),168(g),389(g),171(g),186(v),318(g),393(r)
BD*(2) C12-Zr22	0.07090	-0.01535	
BD*(1) C12-Zr23	0.05293	0.25962	
BD*(1) C12-Zr25	0.02426	0.20015	
BD*(1) C13-Zr19	0.10442	0.18157	155(g),152(g),161(r),150(g),392(g),153(g),291(g),403(v)
BD*(2) C13-Zr19	0.05090	-0.01106	
BD*(1) C13-Zr23	0.05252	0.2651	
BD*(1) C13-Zr24	0.05217	0.26843	
BD*(1) Zr21-H35	0.03795	0.29819	
BD*(1) Zr21-H36	0.03795	0.29819	
BD*(1) Zr23-H37	0.03744	0.31509	
BD*(1) Zr23-H38	0.03744	0.31509	
BD*(1) Zr24-H39	0.03774	0.31342	
BD*(1) Zr24-H40	0.03774	0.31342	
BD*(1) Zr25-H41	0.02631	0.29533	
BD*(1) Zr25-H42	0.02580	0.28437	
BD*(1) Zr25-H43	0.02580	0.28434	

Table 13. NBO data obtained for ZrC nano-sheet.

Bond orbital	Hybrids	occupancy	Energy (a.u.)	Principal Delocalizations (geminal,vicinal,remote)
LP(1) C4	p^{1}	1.08443	-0.13154	128(v),136(v),157(v),118(r),160(v),394(v),203(g),133(v)
LP(1) C5	$sp^{0.26}$	1.93287	-0.49829	137(v),138(v),259(v),380(v), 382(g)
LP*(2) C5	p^{1}	0.41763	-0.10948	134(v),261(v),136(v),208(g)
LP(1) C7	p^{1}	1.07813	-0.13127	145(v),151(r),169(v),172(v),118(r),154(r),406(r),402(v)
LP(1) C8	p^{1}	1.07686	-0.13332	123(v),157(r),151(v),113(r),117(r),154(v),160(r),394(r)
LP*(3) C10	p^{1}	0.61329	-0.09993	134(v),163(r),136(v),261(v),166(r),227(g)
LP(1) C11	$sp^{0.01}$	1.68229	-0.52044	168(r),171(r),398(g),140(v),173(r),318(r),142(v),170(r)
LP*(1) Zr14	$p^{1}d^{18.41}$	0.52930	-0.13087	118(v),127(g),131(r),128(r),147(r),145(r),219(v)
LP*(2) Zr14	$sp^{3.55}d^{1.43}$	0.08110	0.14065	
LP*(3) Zr14	d^{1}	0.06630	-0.12332	
LP*(4) Zr14	$sp^{1.11}d^{1.51}$	0.05044	-0.02547	
LP*(5) Zr14	$p^{1}d^{0.05}$	0.01962	-0.03089	
LP*(1) Zr15	$p^{1}d^{20.57}$	0.52125	-0.12969	113(v),125(r),133(g),123(r),203(v),134(r)
LP*(3) Zr15	$sp^{12.13}d^{3.21}$	0.06205	0.20316	
LP*(5) Zr15	$sp^{0.24}d^{1.15}$	0.02507	-0.05004	
LP*(6) Zr15	$p^{1}d^{0.06}$	0.01702	-0.02474	
LP(1) Zr16	d^{1}	0.87838	-0.10625	115(v),121(v),157(r),208(v), 131(r),227(v),128(r)
LP*(2) Zr16	$sp^{37.59}d^{5.94}$	0.23225	0.20627	130(r),158(r),380(g),382(g),138(g),161(r),259(g),381(v)
LP*(3) Zr16	$p^{1}d^{17.86}$	0.20667	-0.07291	113(v),121(v),115(v)
LP*(5) Zr16	$sp^{0.24}d^{2.41}$	0.01268	0.28256	
LP*(6) Zr16	$sp^{0.5}d^{47.53}$	0.00663	0.35322	
LP*(2) Zr17	$p^{1}d^{20.52}$	0.03212	-0.11491	
LP*(3) Zr17	$sp^{1.34}d^{3.36}$	0.01403	0.02117	
LP*(4) Zr17	$sp^{39.14}d^{16.39}$	0.00749	0.12593	
LP*(5) Zr17	$sp^{7.19}d^{26.54}$	0.00170	0.48873	
LP*(1) Zr18	$p^{1}d^{18.07}$	0.51905	-0.12784	117(v),125(r),149(g),141(r), 123(r),215(v)
LP*(4) Zr18	$sp^{3.38}d^{1.87}$	0.05246	0.02255	
LP*(5) Zr18	$p^{1}d^{0.06}$	0.01987	-0.02952	
LP*(1) Zr19	$sp^{0.02}d^{3.32}$	0.42505	0.12366	392(g),146(r),155(g),405(g), 124(r),291(g),390(v),387(r)
LP*(5) Zr19	$sp^{1}d^{0.05}$	0.07903	0.01102	
LP*(6) Zr19	$sp^{0.01}d^{1.70}$	0.01688	0.19351	
LP*(1) Zr20	$sp^{0.04}d^{3.67}$	0.43730	0.09827	161(g),381(g),393(g),162(r), 124(r),300(g),379(v),391(r)
LP*(2) Zr20	d^{1}	0.28767	-0.08721	113(v),118(r),151(r),
LP*(5) Zr20	$p^{1}d^{0.05}$	0.07839	0.00895	
LP*(6) Zr20	$sp^{0.01}d^{1.92}$	0.01508	0.18303	
LP*(1) Zr21	$sp^{0.15}d^{3.02}$	0.44749	0.09343	397(r),164(g),156(r),395(g),309(g),137(r),159(r),409(g)
LP*(3) Zr21	$sp^{23.76}d^{46.78}$	0.18557	0.05714	162(g),167(g),395(g),156(r),311(g),120(r),137(r),309(g)
LP*(5) Zr21	$p^{1}d^{0.10}$	0.04554	0.09303	
LP*(1) Zr22	$sp^{0.01}d^{3.16}$	0.44506	0.10073	389(g),173(g),401(g),146(r), 140(r),383(r),318(g),387(v)
LP*(5) Zr22	$p^{1}d^{0.05}$	0.04554	0.09303	
LP*(6) Zr22	$sp^{0.01}d^{2.04}$	0.01593	0.21149	
LP*(1) Zr23	d^{1}	0.21798	-0.02355	402(v),406(v),179(r)
LP*(4) Zr23	$p^{1}d^{0.1}$	0.06840	0.09729	
LP*(5) Zr23	$sp^{44.05}d^{41.84}$	0.01931	0.14701	
LP*(3) Zr24	$p^{1}d^{0.17}$	0.07833	0.20896	
LP*(4) Zr24	$p^{1}d^{0.09}$	0.06521	0.09907	
LP*(5) Zr24	$sp^{43.43}d^{41.74}$	0.01823	0.15747	
LP*(1) Zr25	$p^{1}d^{5}$	0.14120	-0.00869	402(v),188(g),417(g),416(g)
LP*(5) Zr25	$p^{1}d^{0.45}$	0.00186	0.08665	

Table 14. NBO data obtained for ZrC nano-sheet.

Bond orbital	Hybrids	occupancy	Energy (a.u.)	Principal Delocalizations (geminal,vicinal,remote)
RY*(3) C1	sp^{1}	0.00024	0.33256	
RY*(4) C1	$sp^{0.11}$	0.00007	0.92498	
RY*(3) C2	p^{1}	0.00041	0.43388	
RY*(4) C2	$sp^{0.01}$	0.00004	1.18757	
RY*(3) C3	p^{1}	0.00042	0.43448	
RY*(4) C3	$sp^{0.01}$	0.00004	1.20722	
RY*(2) C5	$sp^{7.01}$	0.00017	0.77147	
RY*(3) C5	$sp^{0.15}$	0.00006	0.92957	
RY*(3) C7	p^{1}	0.00090	0.52589	
RY*(4) C7	s	0.00009	1.33142	
RY*(1) C8	sp^{1}	0.00260	2.61231	
RY*(3) C9	p^{1}	0.00165	0.56797	
RY*(4) C9	s	0.00009	1.15787	
RY*(3) C10	p^{1}	0.00038	0.48718	
RY*(4) C10	sp^{1}	0.00007	1.13012	
RY*(2) C11	$sp^{50.44}$	0.00150	1.20168	
RY*(3) C12	p^{1}	0.00157	0.55631	
RY*(4) C12	$sp^{0.01}$	0.00013	1.12406	
RY*(1) C13	p^{1}	0.00221	2.22964	
RY*(2) C13	p^{1}	0.00168	0.57304	
RY*(1) Zr14	$sp^{1.27}d^{56.72}$	0.00782	0.36402	
RY*(5) Zr14	$sp^{0.02}d^{0.03}$	0.00063	1.66041	
RY*(6) Zr14	$p^{1}d^{8.72}$	0.00051	0.18271	
RY*(7) Zr14	$sp^{63.63}d^{2.23}$	0.00018	0.96663	
RY*(8) Zr14	$sp^{72.29}d^{1.12}$	0.00013	1.28692	
RY*(9) Zr14	$p^{1}d^{0.11}$	0.00006	0.14785	
RY*(4) Zr15	$p^{1}d^{17.68}$	0.00063	0.20871	
RY*(5) Zr15	$sp^{0.1}d^{0.02}$	0.00035	1.42188	
RY*(6) Zr15	$sp^{11.66}d^{0.34}$	0.00017	0.43745	
RY*(7) Zr15	$p^{1}d^{21.51}$	0.00014	0.20366	
RY*(8) Zr15	$sp^{43.68}d^{2.83}$	0.00011	0.75233	
RY*(9) Zr15	$p^{1}d^{0.1}$	0.00002	0.13125	
RY*(9) Zr15	$sp^{0.42}d^{7.48}$	0.00026	1.70012	
RY*(7) Zr20	$sp^{16.74}d^{0.07}$	0.00013	1.16867	
RY*(8) Zr20	$p^{4.86}d^{0.01}$	0.00004	0.16653	
RY*(9) Zr20	$p^{1}d^{0.04}$	0.00037	0.26992	
RY*(4) Zr21	$p^{1}d^{43.68}$	0.00022	0.26198	
RY*(5) Zr21	$sp^{1}d^{6.91}$	0.00015	1.72160	
RY*(6) Zr21	$sp^{0.02}d^{0.01}$	0.00054	0.31591	
RY*(2) Zr25	$sp^{3.49}d^{44.51}$	0.00024	0.34902	
RY*(3) Zr25	$sp^{0.47}d^{7.32}$	0.00013	0.29668	
RY*(4) Zr25	$p^{1}d^{15.74}$	0.00010	0.20213	
RY*(5) Zr25	$p^{1}d^{8.24}$	0.00007	1.37764	
RY*(6) Zr25	$sp^{0.26}d^{0.13}$	0.00003	0.47172	
RY*(7) Zr25	$sp^{15.90}d^{1.55}$	0.00002	0.85348	
RY*(8) Zr25	$sp^{10.31}d^{0.11}$	0.00084	0.95528	
RY*(1) H26	s	0.00084	0.91930	
RY*(1) H27	s	0.00140	1.33327	
RY*(1) H39	s	0.00140	1.33327	

Table 15. NBO data obtained for ZrC nano-sheet.

Bond orbital	Hybrids	occupancy	Energy (a.u.)	Principal Delocalizations (geminal,vicinal,remote)
CR (1) C1	S	1.99928	-10.0579	129(v),250(v),349(v),252(v),350(v),351(v)
CR (1) C 2	S	1.99919	-10.0587	277(v),241(v),243(v),352(v),353(v),146(v)
CR (1) C 3	S	1.99919	-10.0596	129(v),252(v),243(v),250(v),242(v),130(v)
CR (1) C 4	S	1.99940	-10.0365	130(v),158(v),135(v),296(v),260(v),251(v)
CR (1) C 5	S	1.99986	-10.0997	137(v)
CR (1) C 6	S	1.99921	-10.0683	279(v),143(v),356(v),357(v),148(v)
CR (1) C 7	S	1.99939	-10.0352	150(r),153(r),148(v),152(r),170(v),171(v)
CR (1) C 8	S	1.99937	-10.0357	156(r),159(r),158(r),152(v),124(v),126(v),391(g)
CR (1) C 9	S	1.99945	-10.0062	159(v),295(v),181(v),165(v),158(v),167(v),332(v)
CR (1) C 10	S	1.99959	-10.0748	162(r),397(g),137(v),165(r),139(v),164(r)
CR (1) C 11	S	1.99958	-10.0937	168(r),171(r),140(v),398(g),315(r)
CR (2) Zr 15	P^1	1.99113	-1.25942	376(g),367(g),375(v)
CR (4) Zr 15	P^1	1.99637	-1.30639	113(v),133(g)
CR (3) Zr 17	P^1	1.98472	-1.24792	398(g),400(g),383(g),168(r),171(r)
CR (1) Zr 18	S	1.97949	-2.02139	387(g),384(g),389(v),153(r),372(g),371(v),213(v)
CR (2) Zr 18	P^1	1.99008	-1.25726	372(g),384(g),371(v)
CR (3) Zr 18	P^1	1.98335	-1.24663	387(g),389(v),153(r),384(g),150(r)
CR (4) Zr 18	P^1	1.99607	-1.30455	117(v),149(g)
CR (1) Zr 19	S	1.97309	-1.95986	405(g),239(v),214(r),387(r),392(g),218(v)
CR (2) Zr 19	P^1	1.98709	-1.20913	392(g),390(v),387(r),388(r),158(r)
CR (3) Zr 19	P^1	1.98499	-1.19880	405(g),408(v),407(v)
CR (4) Zr 19	P^1	1.99638	-1.25218	154(g),118(v),117(r)
CR (1) Zr 21	S	1.99048	-1.91981	397(r),396(v),393(v),162(g),120(r),159(r),221(v)
CR (2) Zr 21	P^1	1.98533	-1.17436	395(g),397(r),120(r),393(v),396(v),181(r)
CR (3) Zr 21	P^1	1.98352	-1.17583	409(g),410(g),395(g),120(r),397(r)
CR (4) Zr 21	P^1	1.98354	-1.18374	409(g),410(g),121(r),166(g)
CR (1) Zr 24	S	1.98720	-1.90073	393(v),405(v),407(v),395(v),396(g),159(r),165(r),413(g)
CR (2) Zr 24	P^1	1.98232	-1.16198	396(g),408(g),393(v),405(v),407(v),395(v)
CR (3) Zr 24	P^1	1.98283	-1.16487	413(g),414(g),408(g),396(g),407(v)
CR (4) Zr 24	P^1	1.98546	-1.17348	413(g),414(g),182(g)

CONCLUSION

In this study, from the theoretical analysis of the zirconium carbide nano-sheets, the following were obtained: Polar determinant (Dipole moment, Quadrupole moment, Traceless Quadrupole moment and Octapole moment), EPR data (voltage and voltage difference), NMR parameters (isotropic shielding tensor, anisotropic shielding tensor, asymmetry, span and skew) and NBO data (bonding and anti-bonding orbitals, hybridization of atomic orbitals, energy and Principal Delocalizations).

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