

Geometry Optimization And Energies of Donor-Bridge-Acceptor Molecular System: B3LYP/DFT Calculations

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Abstract:

Theoretical B3LYP/6-31G (d, p) density functional theory has been employed to examine the structural properties of donor-bridge-acceptor molecular system and determine the energies. The electronic states of the system have been calculated depend on Koopman's theorem under the orbital-vertical theory.

The results show that the functional used in the description of the studied molecular system has been proved its validity in calculating the HOMO and LUMO energies and it is a suitable for studying the geometry optimization for the organic molecular system, there are localized orbitals in different parts of the D-B-A molecular system in which that satisfy important property for the D-B-A system to show rectification.

Key words: Donor-Bridge-Acceptor Molecular , B3LYP/DFT Calculations

الامتثلية الهندسية والطاقات للنظام الجزيئي واهب - جسر-قابل: باستخدام حسابات ال B3LYP/DFT

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الخلاصة:

بتطبيق طريقة دالية الكثافة النظرية B3LYP/6-31G (d, P) لفحص الخواص التركيبية للنظام الجزيئي واهب-جسر-قابل وتحديد طاقاته. تم حساب الحالات الالكترونية للنظام قيد الدراسة بالاعتماد على نظرية كوبمان Koopman. تبين النتائج ان الطريقة المستعملة في وصف النظام الجزيئي المدروس قد أثبتت صحتها في حساب طاقات المستوي الجزيئي العلوي المشغول والمستوي الجزيئي السفلي غير المشغول وإنها مناسبة لدراسة الامتثلية الهندسية للأنظمة الجزيئية العضوية، ان للنظام واهب-جسر-قابل مدارات تتوضع في اجزاء مختلفة منه وهذا ما يحقق خاصية مهمة تجعل منه كمقوم.

كلمات مفتاحية: النظام الجزيئي واهب- قابل ، حسابات B3LYP/DFT

Introduction

The main process in many fields of chemistry, physics, and biology [1–7] monographs [8–10] is the charge transfer. This work stand on the design of donor- bridge-acceptor to determine the quantity of charge transfer CT. A convenient model system often used to probe the mechanism of CT in molecular objects with nanoscale dimensions comprises a donor (D) and an acceptor (A) of electrons or holes connected by molecular bridge (B) [11- 17]. The number and variety of such donor-bridge- acceptor (D-B-A) systems have grown explosively in recent years. Molecular bridges linking between an electron donor and an electron acceptor are known to control charge transport in molecular systems. Extensive studies emphasized the role of different factors controlling the charge transport mechanism of donor-bridge- acceptor systems including inter-site electronic coupling, electronic energies and electronic - nuclear coupling. present work focuses on calculating the optimization of the studied structures and energies of donor-bridge-acceptor system and compute the amount of charge transport as a measure the maximum electronic charge that saturates the system, it is a measure of the electronic transfer that a system may accept. The system under study was designed depends on Aviram-Ratner model[18]

Computational Details

Full geometry optimizations of aminobenzene as a donor, nitrobenzene as an acceptor and donor-bridge-acceptor were performed with Berny's optimization algorithm (calculating the energy derivatives with respect to nuclear coordinates analytically [19], in redundant internal coordinates. The gradient corrected density functional methodology was employed: Becke's exchange functional (B) [20] and Becke's three-parameter adiabatic

connection (B3) hybrid [21] exchange functional were used in combination with the Lee–Yang–Parr correlation functional B3LYP [22]. Note that while the BLYP methodology is a 'pure DFT' one (it includes no HF exchange), the B3LYP one contains an admixture of HF exchange (i.e. is of hybrid form). The B3 functional, in fact, contains a linear combination of exact HF exchange, Slater exchange and Becke gradient-corrected exchange [21]. The standard 6-31G(d,p) basis set of DZP quality was used for orbital expansion to solve the Kohn– Sham equations in all cases. Numerical harmonic vibrational analyses were performed for the stationary points found on the potential energy hyper surface, in order to test their character and to compute the harmonic vibration frequencies. The number of imaginary frequencies served as a test whether the stationary points correspond to real minima, or to first-order saddle points. The computed stationary points for which the structures and force fields are presented correspond to real minima on the molecular potential energy hyper surfaces. The DFT (LUMO-HOMO) energy for the donor-bridge-acceptor molecular system studied here was calculated at the same level of theory. All calculations were performed with the GAUSSIAN09 suite of programs [23].

Results and Discussion Geometries

Figure 1 shows the B3LYP/6-31G (d, P) optimized structures. It can be seen from this figure, aminobenzene as a donor and nitrobenzene as an acceptor are connected by (CH)₂ as a bridge. Tables 1, 2 and 3 represent the optimized coordinates for atoms in donor, acceptor and donor- bridge-acceptor, respectively. Tables 4, 5 and 6 show the optimized geometric parameters (bond lengths in angstrom, bond angles in degree and dihedral angles in degree) of donor, acceptor

and donor- bridge- acceptor structures, respectively, calculated by B3LYP/6-31G (d, P) method. It is obvious from table 4 that the geometrical parameters calculations by present method are in good agreement with experimental data for aminobenzene (donor) molecule [24]. The difference of atomic numbers for the conjugated atoms affect on the bond length between these atoms, table 4 declare that the convergence between the bonds C-C and C-N comes from the convergence between their atomic numbers, and this reason explains the difference of C-H bond.

Figure 1: The optimized geometric structures of studied molecules obtained from B3LYP/6-31G (d, p).

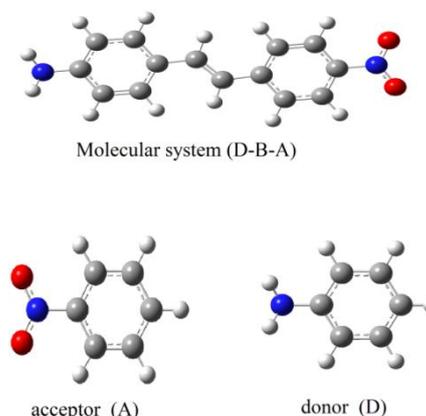


Table 1 : The optimized coordinates of aminobenzene (donor) molecule in (\AA^0) using B3LYP/6-31G (d, p) .

Atom	X (\AA^0)	Y (\AA^0)	Z (\AA^0)
C ₁	1.171292	-1.201966	0.003637
C ₂	-0.221498	-1.207256	-0.005406
C ₃	-0.936853	-0.000042	-0.008519
C ₄	-0.221153	1.207473	-0.005405
C ₅	1.171255	1.201986	0.003616
C ₆	1.880517	-0.000198	0.008312
H ₇	1.704281	-2.145963	0.007358
H ₈	-0.760735	-2.148878	-0.014663
H ₉	-0.760604	2.148987	-0.014839
H ₁₀	1.704695	2.145725	0.007569
H ₁₁	2.963344	-0.000085	0.015667
N ₁₂	-2.337163	0.000030	-0.078638
H ₁₃	-2.776145	-0.833217	0.285928
H ₁₄	-2.776060	0.833252	0.286041

Table 2 : The optimized coordinates of nitrobenzene (acceptor) molecule in (Å^0) using B3LYP/6-31G (d, p) .

Atom	X (Å^0)	Y (Å^0)	Z (Å^0)
C ₁	0.428	1.220	0.000031
C ₂	1.820	1.211222	0.000120
C ₃	2.515501	-0.000018	-0.000005
C ₄	1.820895	-1.211234	-0.000074
C ₅	0.428472	-1.220269	-0.000002
C ₆	-0.242864	0.000047	-0.000075
H ₇	-0.136756	2.141223	-0.000113
H ₈	2.362600	2.149047	0.000239
H ₉	3.598997	-0.000035	0.000051
H ₁₀	2.362517	-2.149087	-0.000169
H ₁₁	-0.136853	-2.141125	0.000087
N ₁₂	-1.718949	0.000009	-0.000021
O ₁₃	-2.290315	-1.086204	0.000124
O ₁₄	-2.290497	1.086131	-0.000066

Table 3 : The optimized coordinates of donor- bridge –acceptor molecular system in (Å^0) using B3LYP/6-31G (d, p) .

Atom	X (Å^0)	Y (Å^0)	Z (Å^0)
C ₁	-4.899924	1.230765	-0.054836
C ₂	-3.517434	1.349168	-0.052496
C ₃	-2.672064	0.224901	-0.003189
C ₄	-3.293385	-1.039015	0.047324
C ₅	-4.671506	-1.169764	0.045552
C ₆	-5.503847	-0.035277	-0.004784
H ₇	-5.519331	2.120181	-0.098995
H ₈	-3.075597	2.339223	-0.089958
H ₉	-2.691007	-1.938037	0.093076
H ₁₀	-5.118546	-2.157711	0.080656
N ₁₁	-6.887122	-0.172766	-0.063403
H ₁₂	-7.260517	-1.035254	0.303624

H ₁₃	-7.422813	0.632856	0.223049
C ₁₄	-1.228630	0.422957	-0.004977
C ₁₅	-0.266938	-0.526281	0.002190
H ₁₆	-0.925668	1.466440	-0.018172
C ₁₇	1.174958	-0.302982	0.003642
C ₁₈	1.770377	0.976604	0.044237
C ₁₉	3.146498	1.131482	0.042204
C ₂₀	3.959527	-0.003246	0.000483
C ₂₁	3.413263	-1.284374	-0.038311
C ₂₂	2.032849	-1.422154	-0.035741
H ₂₃	1.151030	1.863284	0.081863
H ₂₄	3.602645	2.110664	0.073895
H ₂₅	4.068142	-2.143399	-0.069605
H ₂₆	1.601275	-2.416037	-0.066279
N ₂₇	5.414575	0.157026	-0.000551
O ₂₈	6.106258	-0.859911	-0.036480
O ₂₉	5.868182	1.300311	0.034631
H ₃₀	-0.559756	-1.571957	0.001524

Table 4: The optimized geometric parameters (lengths in angstrom , angles in degree and dihedral angles in degree) of aminobenzene (D) using B3LYP/6-31G (d ,p).

Bond Length (Å ⁰)		Bond Angle (deg)		Dihedral angle (deg)	
Bond	Value	Bond	Value	Bond	Value
R(c-c)	1.392	A(c-c=c)	120.765	D(c=c-c=c)	-0.069
R(c-H)	1.084	A(c-c-H)	119.232	D(H-c-c=c)	179.911
R(c=c)	1.403	A(c=c-H)	120.002	D(H-c-c-H)	-0.366
R(N-H)	1.009	A(c=c-c)	118.694	D(c-c=c-c)	0.142
		A(c=c-N)	120.617	D(c-c=c-N)	177.100
		A(c-N-H)	114.584	D(H-c=c-N)	-2.622
		A(H-N-H)	111.190	D(N-c-c=c)	-177.099
				D(N-c-c-H)	2.611
				D(c=c-N-H)	156.683

Table 5: optimized geometric parameters (lengths in angstrom, angles in degree and dihedral angles in degree) of nitrobenzene (A) using B3LYP/6-31G (d, p).

Bond Length (Å ⁰)		Bond Angle (deg)		Dihedral angle (deg)	
Bond	Value	Bond	Value	Bond	Value
R(c=c)	1.392	A(c=c-c)	118.443	D(c-c=c-c)	0.010
R(c-H)	1.080	A(c=c-H)	121.917	D(c-c=c-H)	180.005
R(c-N)	1.476	A(c-c-H)	119.640	D(H-c=c-c)	180.010
R(N-O)	1.227	A(c=c-c)	120.206	D(H-c=c-H)	0.004
		A(c-c=c)	122.365	D(c-c-c-c)	-0.0091
		A(c-c-N)	118.819	D(c=c-c=c)	-0.001
		A(c-N-O)	117.746	D(c=c-c-N)	-180.009
		A(O-N-O)	124.500	D(H-c-c-c)	179.998

Table 6: optimized geometric parameters (lengths in angstrom, angles in degree and dihedral angles in degree) of donor- bridge- acceptor (D-B-A) system using B3LYP/6-31G (d, p).

Bond Length (Å ⁰)		Dihedral angle (deg)		Dihedral angle (deg)	
Bond	Value	Bond	Value	Bond	Value
R(c=c)	1.403	D(c=c-c-H)	-179.889	D(c-c-c=c)	0.158
R(c-H)	1.084	D(H-c-c-H)	0.322	D(c-c=c-H)	0.018
R(c-N)	1.391	D(c-c=c-c)	-0.082	D(c-c=c-c)	0.035
R(N-H)	1.009	D(c-c=c-N)	-177.258	D(N-c=c-H)	-0.057
R(c-c)	1.411	D(H-c=c-N)	2.530	D(c-c-N-O)	-0.065
R(N-O)	1.230	D(H-c=c-c)	-0.049	D(c=c-c-c)	0.062
		D(c=c-c=c)	-178.100		
		D(H-c=c-H)	-0.534		
		D(c=c-c-N)	177.268		
		D(H-c-c-N)	-2.567		
		D(c=c-N-H)	-23.500		
		D(c-c-N-H)	24.217		
		D(c-c=c-H)	0.530		
		D(c=c-c-c)	2.279		
		D(H-c-c=c)	1.841		
		D(c-c-c-H)	0.315		

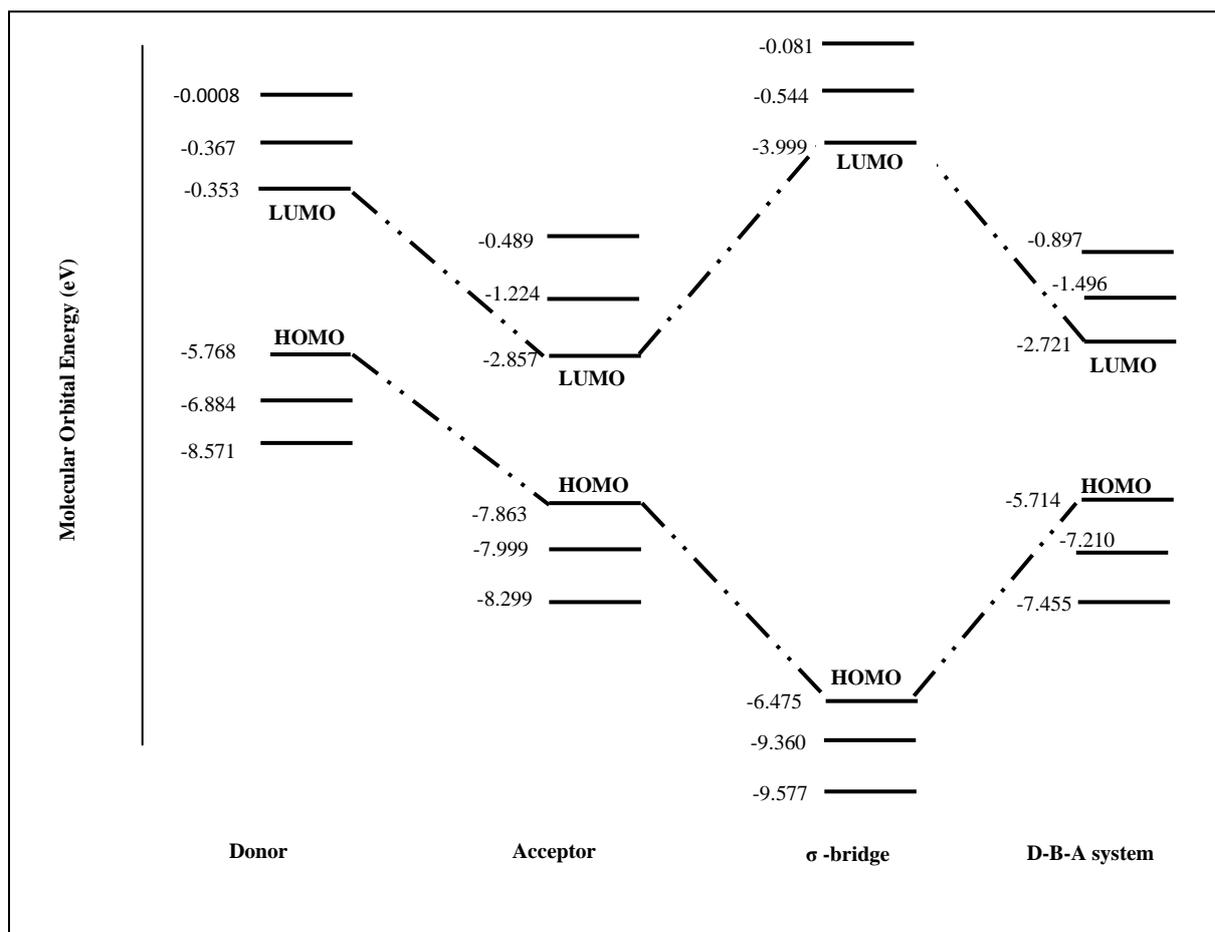


Figure 7: Energy level diagram for donor, bridge, acceptor and D-B-A molecular system.

It is clear from table 1 that the geometrical parameters calculations in present study are in a good agreement with experimental data.

Table 6 shows that the optimized bond lengths of the bridge backbone linking between donor and acceptor are having double bond less than 1.35 \AA , and it can be seen that a minor deviation in the bridge bond angle and dihedral angle between the two planes

containing the end substituent's. This deviation can be expected due to strict interaction coming from the presence of phenyl groups at the terminal positions.

Table 7 shows the results of total energy E_{tot} , variational ratio $(-V/T)$, symmetry and number of imaginary frequency for aminobenzene (D), nitrobenzene (A), $(CH)_2$ (B) and D-B-A molecules obtained from B3LYP/6-31G (d, p) calculations.

Table 7: Total energy in (a.u), ($-V/T$), symmetry and number of imaginary frequency for studied molecules from B3LYP/6-31G (d , p) functional.

Species	E_T (a.u)	($-V/T$)	Symmetry	NO. Of imaginary frequency
Donor (D)	-287.647	2.008	C_s	0
Bridge (B)	-76.216	2.008	C_{2h}	0
Acceptor (A)	-436.803	2.007	C_{2v}	0
Molecular System (D-B-A)	-800.670	2.007	C_1	0

It is obvious from table 7 that the total energy for D-B-A system is less than the total energy of mentioned molecules in this study, the total energy of D-B-A system is approximately the summation of total energy for all donor, bridge and acceptor molecules, as illustrated in figure 2 it can be found an equation associates the total energy E_T for the donor- bridge –acceptor molecular system with its components:

$$E_T(\text{system}) \cong E_T(D) + E_T(B) + E_T(A)$$

From table 7, one can see that all structures have not imaginary frequency, this may refers to that 6-31G (d, p) is a suitable level of theory used in optimization geometry for this type of structures. Table 7 shows also the symmetry of studied molecules, aminobenzene (donor) is a planar and has a low symmetry, nitrobenzene (acceptor) has high symmetry and the donor- bridge- acceptor molecular system has C_1 symmetry and this means that only a rotation of 360° leaves it apparently unchanged.

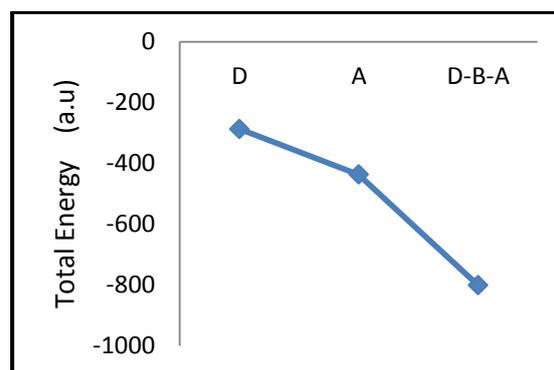


Figure 2: The total energy for donor, acceptor and donor – bridge - acceptor system by B3LYP/ 6-31G (d, p).

Electronic States and Energy Gap

Table 8 shows the high occupied molecular orbital energy E_{HOMO} lower unoccupied molecular orbital energy E_{LUMO} , and energy gap E_g for donor, acceptor, and donor- bridge –acceptor molecules. It has been found that the bridge $(CH)_2$ used to link the aminobenzene as a donor with nitrobenzene as an acceptor gave a new structure as a donor- bridge – acceptor system has a small energy gap in compared with donor and acceptor, the energy gap for D-B-A system is 2.993 eV. Figure 3 shows the energy gap for studied molecules.

Table 8: E_{HOMO} , E_{LUMO} and energy gap E_g for donor, acceptor and donor – bridge –acceptor molecular system.

Species	$E_{HOMO}(ev)$	$E_{LUMO}(ev)$	$E_g (ev)$
Donor (D)	-5.768	-0.353	5.415
Acceptor (A)	-7.863	-2.857	5.006
Molecular System (D-B-A)	-5.714	-2.721	2.993

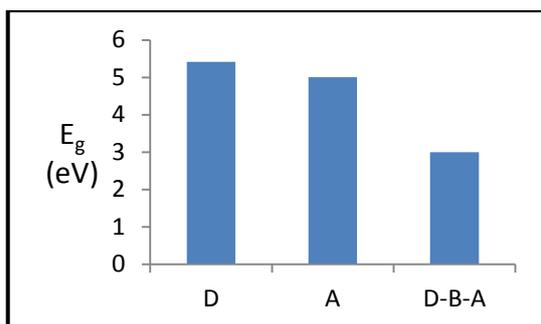


Figure 3: Energy gap for donor, acceptor, and donor- bridge- acceptor molecular system.

The interaction between aminobenzene (D) and nitrobenzene (A) through the bridge affected on HOMO and LUMO of these molecules, the main change occurs at LUMO of the donor and HOMO of the acceptor and this change depends on the type of bridge used in linking donor and acceptor. Figures 4, 5 and 6 show the LUMO- HOMO for donor, acceptor and D-B-A system, respectively. And figure 8 shows the shapes of HOMO and LUMO for these structures, drawn by Gaussian View 5.0.8 using B3LYP/6-31G (d, p) method.

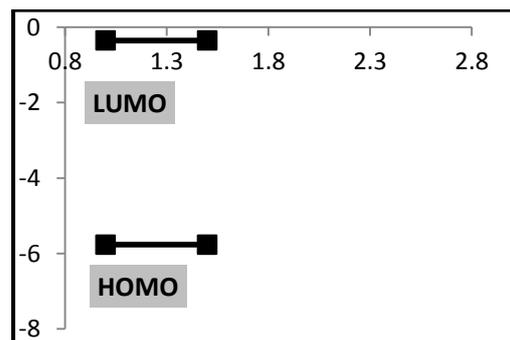


Figure 4: LUMO-HOMO energy for aminobenzene (D).

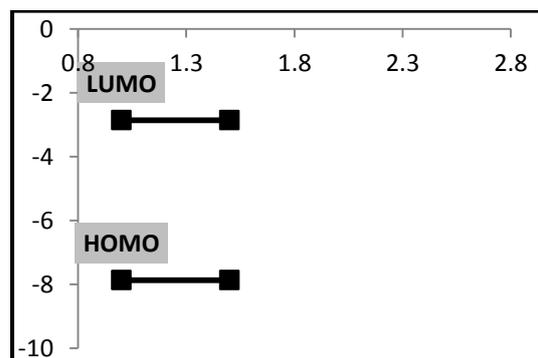


Figure 5: LUMO-HOMO energy for nitrobenzene (A).

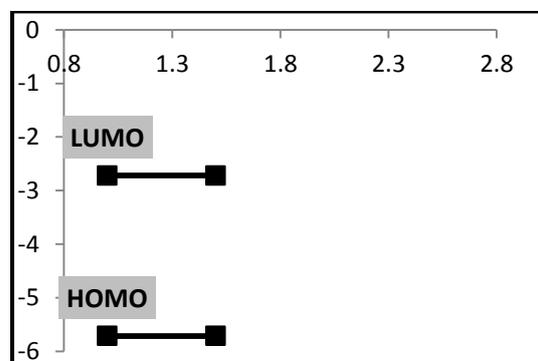


Figure 6: LUMO-HOMO energy for D-B-A system.

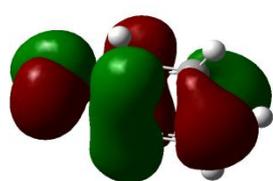
In this system, the donor part and acceptor part are coupled through σ -bridge to result the molecular system. As we know that the structural construction principle of organic molecular rectifier is based on acceptor part and donor part connected through an insulating bridge, these three (donor, acceptor and bridge) can be considered as components in bringing out the rectifier.

The optimization of donor, acceptor, σ -bridge and D-B-A molecular system has been carried out at B3LYP/6-31 G(d, p) level along with the population analysis and donor for comparison analysis of the energy level arrangements in these components and the system.

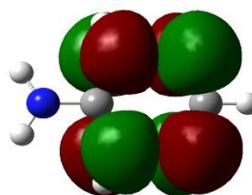
Figure 7 shows the energy level diagram for the three highest occupied and three lowest unoccupied molecular orbitals for the donor, bridge, acceptor and D-B-A system. From this diagram, one can see that the HOMO and LUMO for the acceptor are more stable in comparison with donor. The HOMO and LUMO for donor are

situated (-5.768, -0.353) eV, higher than the HOMO and LUMO for acceptor, but (LUMO-HOMO) for both donor and acceptor is approximately the same (5.415 eV for donor and 5.006 eV for acceptor). The electron injection of an electron to the LUMO of the acceptor will be a lower energy process compared to the donor because the LUMO of the acceptor is more stable in compared to donor. On the other hand, removal of one electron from the HOMO of the donor will be a less energetic process compared to the acceptor because the HOMO of the donor is less stable in compared to HOMO of the acceptor.

The energy level diagram shows that the HOMO of σ -bridge (-6.475 eV) is more stable like the HOMO of the acceptor and the LUMO (-3.999 eV) is unstable like the LUMO of the donor, and σ -bridge has very high energy gap in which this indicate that σ -bridge can acts as a suitable barrier. The (LUMO-HOMO) for the D-B-A is small (2.993eV) in compared to donor, bridge and acceptor.

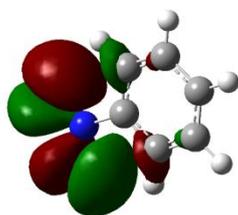


LUMO

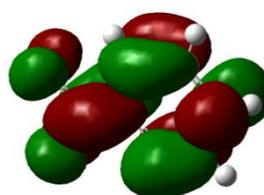


HOMO

Donor

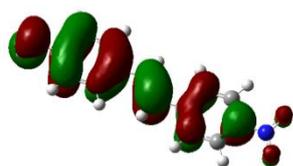


LUMO

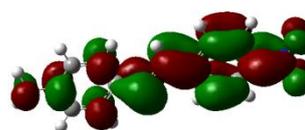


HOMO

Acceptor



LUMO



HOMO

D-B-A system

Figure 8: The shapes of HOMO and LUMO for studied structures.

Conclusions

1. B3LYP/6-31 G(d, p) density functional theory has been proved its validity in studying the geometry optimization and calculating the geometrical parameters. Therefore, density functional theory presented good results in calculation of total energy for the D-B-A molecular system comes from the summation of total energies for all donor, bridge and acceptor parts.
2. The large 6-31 G(d, p) basis set used to describe the studied structures with B3LYP functional level is a significant theory for calculating the electronic states (HOMO and LUMO) and studying the spectra analysis for the studied molecular electronics, but it requires a large time compared with other small basis sets.
3. The presence of substituents in phenyl rings at the donor and the acceptor did not have effect on the

aromaticity of these organic molecules. So, the aromaticity of phenylenes keep under the connection donor part and acceptor part through the σ -bridge.

4. Phenyl ring with amino group was truly predicted to be a better semiconducting material because of its lower oxidation potential, it is good electron donating group.
5. Small value of (LUMO-HOMO) for the D-B-A molecular system compared with their individual components. For device application with these structures connected to two electrodes, a decrease in (LUMO-HOMO) value is playing an important role in electron injection.
6. From the molecular orbital distribution, there are localized orbitals in different parts of the D-B-A molecular system in which that satisfies important property for the D-B-A system to show rectification.

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