

Quantum chemical studies of nitrogen substitution on ZnO nanoclusters stability

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ABSTRACT

Importance of p-type transparent conducting oxide (TCO) is much needed in the optoelectronics industry. Due to lack of intrinsic p-type TCO, it is necessary to design or tune the properties existing n-type TCO are very essential. This present work describes, n-type ZnO is tuned to p-type by doping of nitrogen on to the nanocluster. The structural stability of $Zn_xO_{x-1}N$ for $x=(2-5)$ is optimized using Gaussian 09 program package with a B3LYP/6-31G level basis set. The optimization result shows that when the cluster size increases the stability also increases. The dipole moment depends on the structure of the $Zn_xO_{x-1}N$ cluster. These optimized structural geometries are used to calculate the binding energy, HOMO-LUMO energy gap, ionization potential and electron affinity of nanoclusters. The binding energy for ring structures is found to be more than the other two structures. Vibrational analysis is carried out for all the structures and reported. The ring structure is found to be more stable than the linear and 3D structures. The findings of the present work will provide an insight to synthesis, p-type ZnO nanoclusters. Copyright © 2015 VBRI Press.

Keywords: Nanocluster; ZnO:N; DFT; binding energy; structural stability.



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Introduction

Zinc Oxide is an n-type semiconductor with wide bandgap of 3.37 eV, which exhibits wurzite structure. ZnO in its wurzite lattice belongs to P63mc space group which is characterized by two interconnecting sublattices of Zn^{2+} and O^{2-} where zinc ion is surrounded by a tetrahedral oxygen ions and vice-versa. The n-type behavior is due to the metal rich and oxygen deficient. Nowadays, significant works are going on towards the fabrication of p-type ZnO which has potential applications in laser and ultraviolet light emitting diodes [1]. For the preparation of p-type ZnO, nitrogen is doped, due to its low ionization energy, ionic radius, easy availability, low toxicity and easy handling. ZnO is widely used in optoelectronic devices such as photodetectors, gas sensors, light-emitting diodes, varistors, piezoelectric devices, batteries, fuel cells, photocells and catalyst [2-8]. ZnO is a very good functional material with diverse growth morphologies such as nanowire, nanocombs, nanoflower, nanorings, nanobelts, nanocages etc. Many works have been reported on theoretical studies in ZnO nanoclusters [9-11]. One of the mechanisms widely used in research field is to convert n-type ZnO to p-type by implanting nitrogen ion on the structure of ZnO [12-17]. From the survey, it is known that much work has not been carried out based on density functional theory (DFT) approach for nitrogen substituted ZnO clusters. DFT is preferable for application in the materials science since it can handle bulk as well as the

structural calculations [18]. One of the major advantages of DFT is to tailor the properties of materials without feeding the experimental data with low computational cost compared to other calculation method [19]. The objective of the present work is to study the structural stability of ZnO nanoclusters with the incorporation of nitrogen as an impurity. The novel aspect of the present work is to enhance the p-type behavior of ZnO nanoclusters with the incorporation of N atoms in the cluster. In the present work, $Zn_xO_{x-1}N$ nanoclusters are simulated up to $x=2-5$ for three different structures (linear, ring and 3D) and their structural stability, dipole moment, HOMO-LUMO energy gap, binding energy, Ionization Potential (IP) and Electron affinity (EA) have been calculated and reported.

Computational details

The clusters of nitrogen substituted Zinc Oxide ($Zn_xO_{x-1}N$) for $x=2-5$ are simulated through Gaussian 09 package [20]. The energy minimization and dipole moment have been calculated by the simulation with Becke's three-parameter hybrid functional combined with Lee-Yang-Parr correlation functional (B3LYP) method together with the 6-31G basis set [21-25]. Since Zinc, Oxygen and Nitrogen have atomic numbers of 30, 8 and 7 respectively, 6-31G basis set [26] has been used to compute the minimum energy and dipole moment. GaussSum 3.0 [27] is used to plot density of states (DOS) spectrum from the Gaussian output.

Results and discussion

Structures of $Zn_xO_{x-1}N$ clusters

The calculated energy, dipole moment values and point group of $Zn_xO_{x-1}N$ clusters for ($x=2-5$) are shown in **Table 1**.

Table 1. Energy and dipole moment of $Zn_xO_{x-1}N$ clusters ($x=2$ to 5).

Model	Cluster Size	Energy (Hartrees)	Dipole Moment (Debye)	Point Group
linear	2	-3688.024	2.8544	$C_{\infty V}$
	3	-5542.396	3.3524	$C_{\infty V}$
	4	-7396.747	3.3167	C_S
	5	-9251.080	3.4024	$C_{\infty V}$
ring	2	-3688.018	0.8196	C_S
	3	-5542.243	1.0773	C_S
	4	-7396.565	2.2901	C_S
3D	5	-9251.126	1.1315	C_S
	3	-5542.405	5.8552	C_S
	4	-7396.780	0.1590	C_1
	5	-9251.081	5.1544	C_1

From the tabulated values it is seen that, irrespective of the model, the energy decreases when the cluster size increases infer that when the number of atoms is added to the cluster the stability increases. From the obtained computed energy values, all the structures of Zn_5O_4N have less energy and it is most stable. The possible structural diagrams of $Zn_xO_{x-1}N$ clusters for ($x=2-5$) are shown in **Fig 1(a) - (c)**. The Zn_2O_1N cluster has two isomers (**Fig 1(a)** and **(b)**) of linear and ring structures respectively. In these two isomers, the ring structure has lower energy and square planar geometry. The bond length between N and Zn atom in linear structure is about 1.7Å whereas it is optimized in the ring structure with 1.9Å.

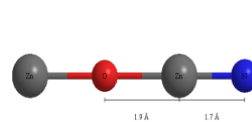


Fig. 1(a)

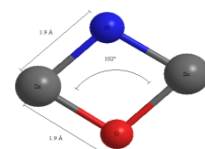


Fig. 1(b)

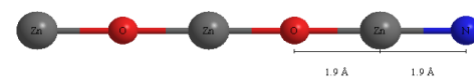


Fig. 2(a)

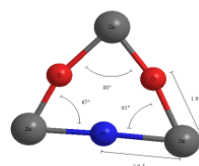


Fig. 2(b)

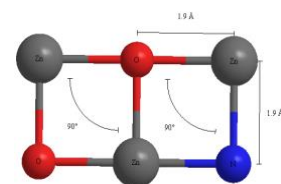


Fig. 2(c)

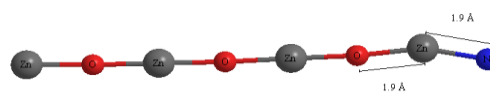


Fig. 3(a)

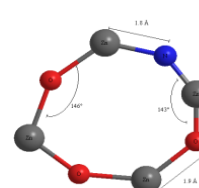


Fig. 3(b)

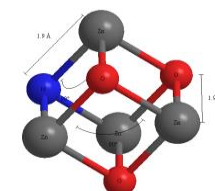


Fig. 3(c)

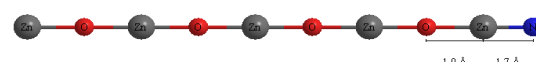


Fig. 4(a)

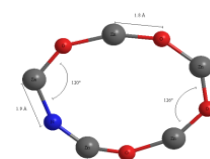


Fig. 4(b)

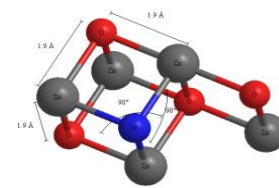


Fig. 4(c)

Fig. 1-4 B3LYP/6-31G optimized geometrical structures of $Zn_xO_{x-1}N$.

The variation in bond length and the type of the structure makes the angle between Zn-O-Zn is about 102°. There are three possible isomers constructed for Zn_3O_2N cluster shown in **Fig 2(a) – Fig 2(c)**. Among the three structures the 3D model has the energy difference of -0.009 Hartrees and -0.162 Hartrees with linear and ring structures

since it resembles the closed cubic structure. The optimized bond length between Zn-N and Zn-O is about 1.9 Å for linear and 3D structures and in the case of a ring, the bond length between Zn-N is optimized to 2.0 Å. For Zn_4O_3N with three different isomers, the 3D structure has less energy than the other two. The energy difference between 3D and Linear is about 0.033 Hartrees with the equal bond lengths. In ring structure the bond length between Zn-O and Zn-N is 1.9 Å and 1.8 Å respectively and the angle between O-Zn-N is about 143°. The Zn_5O_4N cluster has three isomers, among these; the ring structure has higher stability than the linear and 3D structures with the energy difference 0.045 Hartrees and 0.046 Hartrees respectively.

The dipole moment obtained for $Zn_xO_{x-1}N$ ($x=2-5$) clusters shows that the ring structure has lesser values due to neutralization of charges in the atoms since it has closed structure. In 3D structures, only Zn_4O_3N has the least value because it has completely closed cubic structure. For linear structures the dipole moment varies randomly due to unequal charge present in the cluster and it shows an increasing trend due to the cluster size. The point group for linear structure for $x=2, 3$ and 5 is $C_{\infty V}$ which has high order of asymmetry due to the position of atoms in the cluster. For linear structure the point group is $C_{\infty V}$ or C_s . Due to the closed ring structures the point group for all the clusters in this group is C_s . However, in the case of 3D structure the point group is C_s or C_1 , the dipole moment variation in this 3D structure is due to the positioning of the atoms.

Binding energy of $Zn_xO_{x-1}N$ clusters

The relative stabilities of $Zn_xO_{x-1}N$ ($x=2-5$) clusters are determined based on the binding energy per atom in the cluster using the following formula

$$E_{BE} = (n \cdot E(Zn) + m \cdot E(O) + E(N) - E(Zn_nO_mN)) / (n + m + 1)$$

Where, n is the number of Zn atom and m is the number of O atom. The calculated binding energies of $Zn_xO_{x-1}N$ are tabulated in **Table 2**. From the calculated E_{BE} values it is observed that compared to linear and 3D structures, the ring structure is stable since it has higher binding energy [28]. It may be due to the position of the atom in the cluster, bond length between the atoms in the cluster. The random variation in the binding energies of all the structures depends upon the placement of atoms in the clusters. Among all the clusters, Zn_3O_2N has high binding energy value of 0.6775 eV, since the bond lengths are almost equal.

Table 2. Binding energies of $Zn_xO_{x-1}N$ ($x=2-5$) nano clusters.

Cluster Size	linear (eV)	ring (eV)	3D (eV)
2	0.5088	0.5496	-
3	0.0136	0.6775	0.0517
4	0.2040	0.4136	0.3156
5	0.2693	0.3945	0.2748

HOMO and LUMO analysis

The chances in the chemical reaction will depend on the HOMO-LUMO energy gap [29-32]. When the cluster size increases due to accommodation of more number of atoms the energy gap reduces in the cluster. Comparing the energy gap with all the structures, for linear structures there is a consistent decrease in the gap with cluster size and has more energy gap than that of ring and 3D structure since in the linear structure, the structure gets truncated. The density of states spectrum and HOMO-LUMO energies of Zn_5O_4N structure for linear, ring and 3D structure are shown in the **Fig. 5(a)**, **(b)** and **(c)** respectively.

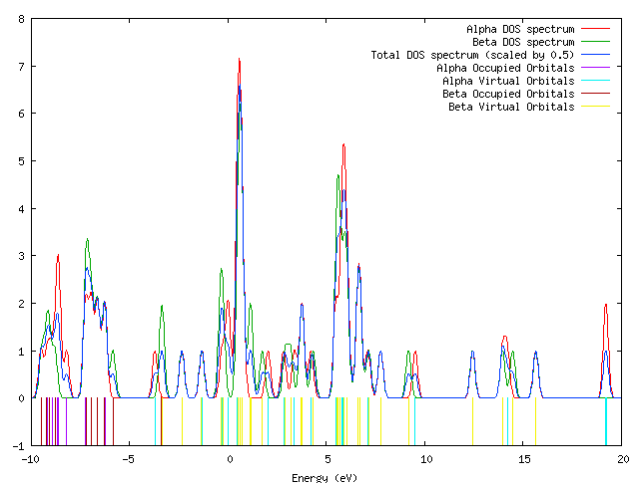


Fig 5. (a) HOMO-LUMO, DOS spectrum of Zn_5O_4N nanocluster linear structure.

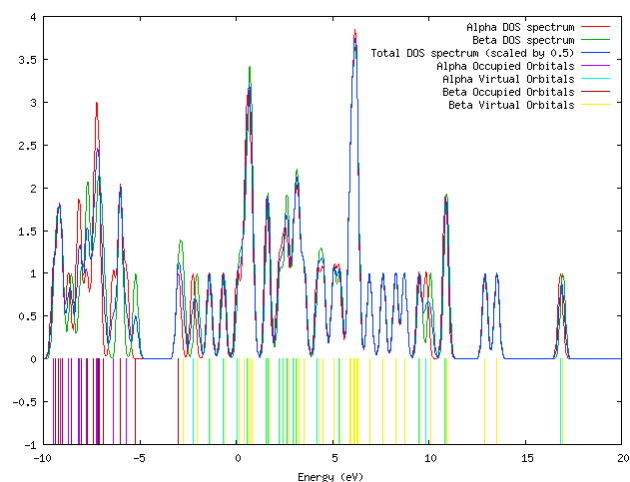


Fig 5. (b) HOMO-LUMO, DOS spectrum of Zn_5O_4N nanocluster ring structure.

From the DOS spectra of Zn_5O_4N linear, ring and 3D structures as in **Fig 5(a)**, **5(b)** and **5(c)**, it is observed that the acceptor level is very low in the linear structure compared to the other two structures (ring and 3D). This indicates that, for closed structures of nitrogen doped ZnO, the acceptor level will be more so that one can expect the stable p-type conductivity. The increase in the cluster size results in the delocalization of valence electrons over number of atoms in the cluster. The HOMO-LUMO visualization and their spin states are tabulated in **Table 4**.

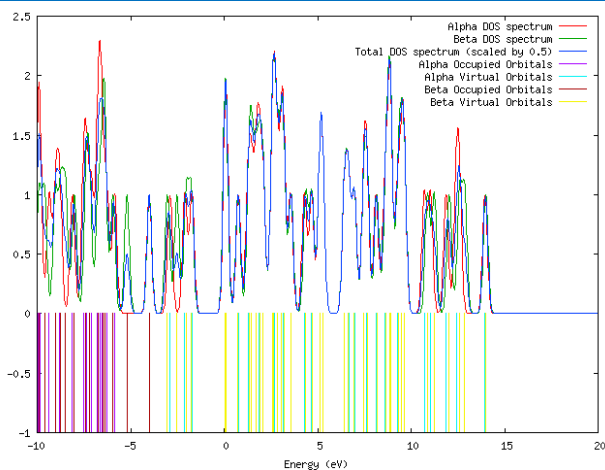


Fig 5. (c) HOMO-LUMO, DOS spectrum of Zn_5O_4N nanocluster 3D structure

Table 3. HOMO-LUMO gap of $Zn_xO_{x-1}N$ ($x=2-5$) nano clusters.

Structure	Size	HOMO Alpha (eV)	LUMO Alpha (eV)	Gap (eV)	HOMO Beta (eV)	LUMO Beta (eV)	Gap (eV)
linear	2	-6.86	-3.7	3.16	-5.88	-3.25	2.63
	3	-6.46	-3.69	2.77	-5.82	-3.03	2.79
	4	-6.28	-3.62	2.66	-5.8	-3.02	2.78
	5	-6.27	-3.72	2.55	-5.85	-3.39	2.46
ring	2	-6.46	-3.66	2.8	-5.28	-3.15	2.13
	3	-4.81	-3.79	1.02	-5.11	-3.42	1.69
	4	-5.64	-4.22	1.42	-4.79	-4.31	0.48
	5	-5.69	-3	2.69	-5.22	-2.99	2.23
3D	3	-6.06	-3.46	2.6	-5.4	-3.32	2.08
	4	-6.08	-3.29	2.79	-5.79	-3.27	2.52
	5	-5.86	-4.01	1.85	-5.19	-4	1.19

Table 4. HOMO-LUMO visualization and spin states of $Zn_xO_{x-1}N$ clusters.

Cluster	Spin State	HOMO	LUMO
Zn_2O_1N linear	Singlet		
Zn_2O_1N ring	Singlet		
Zn_3O_2N linear	Doublet		
Zn_3O_2N ring	Quartet		

Zn_3O_2N 3D	Doublet		
Zn_4O_3N linear	Octet		
Zn_4O_3N ring	Doublet		
Zn_4O_3N 3D	Doublet		
Zn_5O_4N linear	Doublet		
Zn_5O_4N ring	Doublet		
Zn_5O_4N 3D	Doublet		

Ionization potential and electron affinity

The study of ionization potential (IP) and electron affinity (EA) are very important for nanoclusters since they indicate the electronic structure of the clusters and also a measuring tool for individual atomic to bulk behavior change [4]. Ionization potential and electron affinities of different isomers provide important clues for identifying various low energy isomers. The IP and EA values for $Zn_xO_{x-1}N$ clusters are calculated from their orbital energies. The variation of ionization potential and electron affinities of linear, ring and 3D structures with cluster size is shown in the **Fig. 6(a), (b)** and **(c)**, respectively.

For linear structure, the ionization potential and electron affinity are found to be almost the same value since all the atoms are connected as a chain and are having an energy difference of approximately 0.2 eV. Besides, in the case of ring structure the ionization potential and electron affinities vary in a zig-zag path, due to the formation of closed structure.

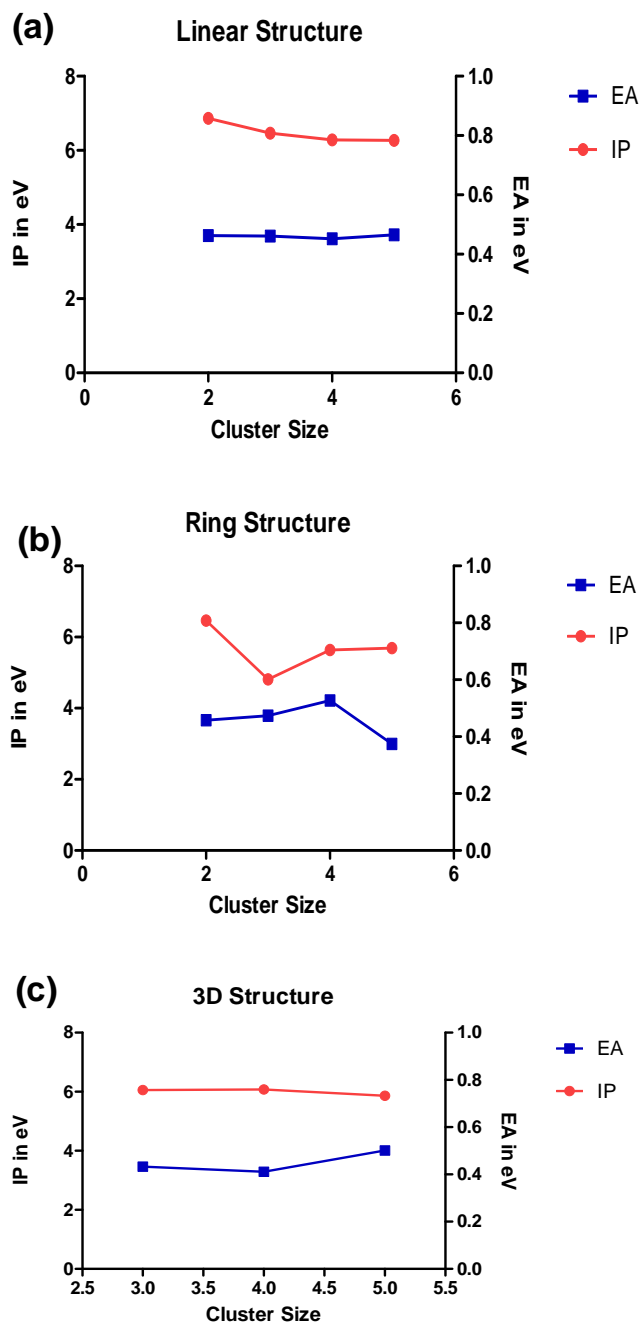


Fig 6. (a) IP and EA of Zn_xO_{x-1}N clusters –Linear Structure (b) IP and EA of Zn_xO_{x-1}N clusters –ring structure, and (c) IP and EA of Zn_xO_{x-1}N clusters –3D structure.

In the case of 3D clusters, the atoms in the clusters are held compact, which has a trend of almost the same value of the ionization potential and electron affinity. The cluster with high value of electron affinity is more preferable for chemical sensors. Among all the clusters, EA value is high of about 4.22 eV for ring structured Zn₅O₄N. If a proper cluster could be synthesized in the 3D structure, then those can be easily utilized in the chemical sensors. The large value of electron affinity infers that it is more chemically reactive. Interestingly, the electron affinity for linear structure is observed to be high, which is chemically reactive than the other two structures namely linear and 3D structures.

Vibrational mode analysis

Analysis of the normal vibrational modes of isomers is carried out and tabulated in **Table 5**. The vibrational study is used to predict the stability of the low lying isomers for Zn_xO_{x-1}N clusters [33, 34]. In the case of ring structure the maximum and minimum infrared (IR) intensity are observed, the IR intensity for x=2 ring structure is found to be 64.9955 km mole⁻¹ whereas the IR intensity for x=4 and x=5 in the ring structure is 0.0026 and 0.0001 km mole⁻¹ respectively. In contrast, for 3D structure the IR intensity is 8.3521, 1.144 and 4.801 km mole⁻¹ for x=3, 4, 5 respectively, all the modes are only due to molecular twist. Simulated IR spectra for the stable ring structures(x=2-5) are shown in **Fig 7**.

Table 5. Vibrational mode assignments for Zn_xO_{x-1}N clusters.

Structure	Cluster size	Vibrational frequency (cm ⁻¹)	IR intensity km mole ⁻¹	Mode Assignment
linear	2	43.2697	1.6012	Zn-O Stretching
	3	91.0235	21.4893	Zn-O Bending
	4	56.4751	12.4568	Zn-O Bending
	5	62.8460	5.9400	Zn-O Bending
ring	2	85.6462	64.9955	Zn-N Stretching
	3	64.4718	8.3058	Molecular twist
	4	73.5810	0.0026	Zn-O Stretching
	5	42.9501	0.0001	Molecular twist
3D	3	64.9503	8.3521	Molecular twist
	4	149.453	1.1440	Molecular twist
	5	79.2572	4.8401	Molecular twist

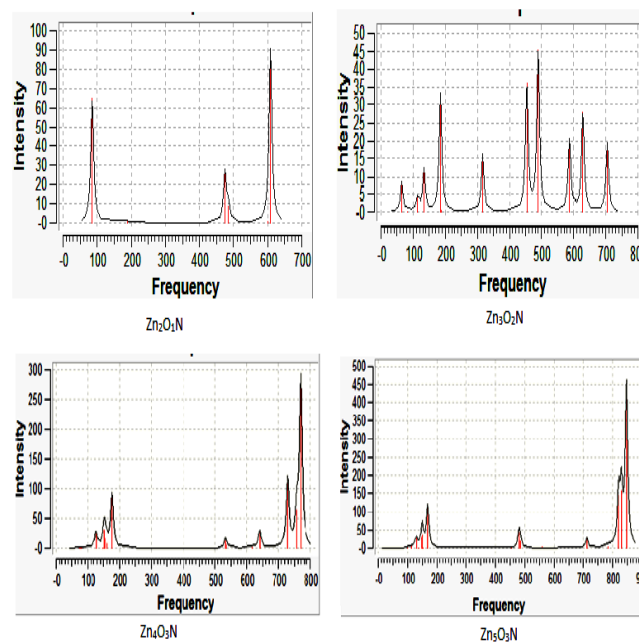


Fig 7. Simulated IR Spectra for ring structures Zn_xO_{x-1}N(x=2-5).

Conclusion

The nitrogen substituted ZnO clusters have been completely optimized with the B3LYP/6-31 G basis set.

The observed results show that the closed ring structures are more stable than the other two structures. The stability of the clusters increases with the cluster size. The dipole moments for different structures depend on the position of the atoms in the cluster. The calculated binding also shows that the ring structured isomers are more stable than the other two structures. The ionization potential for linear structures are high, hence chemically reactive and electron affinity for all the clusters are almost the same value except for ring structured Zn_4O_3N . HOMO-LUMO energy gap reveals that when the atoms in the cluster increase the energy gap decrease which reflects the overlapping of the orbitals due to the increase in the number of atoms. From the density of states analysis, compared to linear structures, the closed structures such as ring and 3D possess more p-type conductivity. Vibrational analysis shows that the IR intensity is found to be maximum and minimum for ring structure. The findings of the present work provide the insight to experimentalists for tailoring a new material which suits for the development of p-type ZnO with nitrogen substitution.

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