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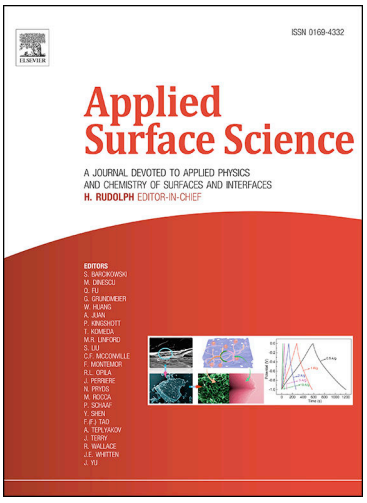

Full Length Article

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Ab initio study of hydrogen sensing in Pd and Pt functionalized GaN [0001] nanowires

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Abstract

Using density functional theory based simulations, the adsorption of hydrogen on GaN nanowires with [0001] orientation is studied with Pt and Pd functionalization. The adsorption energies show that both Pt and Pd prefer to attach to a top site above the Ga atom in the nanowire. In the pristine GaN, hydrogen attach as a molecule, while in the presence of Pt and Pd, it dissociates into atoms and adsorb through a chemical bonding. Change in Ga-N bond lengths are observed with hydrogen adsorption on the surface of the nanowire and the resultant strain as well as the charge transfer between atoms can be used as entities to understand the detection mechanism. From the electronic structure analysis, it is revealed that both Pt and Pd can be used to tune the band gap and are favorable adsorbates to enhance the hydrogen sensing properties of GaN nanowires. Pt turns out to be a more efficient adsorbate for hydrogen detection due to the lowered adsorption energies, compact Pt-H bond length and enhanced surface charge reconstruction.

Key words: GaN nanowire, H_2 sensing, metal functionalization, adsorption energy, electronic structure

Introduction

Dilute magnetic semiconductors (DMSs) in general and GaN in specific is exceptional owing to the wide and direct band gap, heat resistance, large surface to volume ratio as well as strong chemical stability which makes it potential candidate for many applications [1-3]. One interesting aspect about DMS materials is that their properties can be modulated in various dimensions such as bulk, 2D materials, nanowires and nanoclusters [4-8]. In this scenario, nanowires of GaN are versatile in their functionalities and for utilizing them for gas sensing applications, it is very important to understand the mechanism of adsorption and subsequent interaction of gas phase atoms with the nanowire surface [9]. Furthermore, the adsorbates are known to influence valence band bending at the surface [10]. The use of transition metals (TMs) to functionalize the GaN nanowires and further H_2 sensing mechanism has been investigated in extant literature [11,12]. By metal functionalization, the band gap of GaN nanowires can be tuned. Visible changes can also happen in the absorption spectra of the nanowires owing to the adsorption of metals [13]. Most of the TM family has been used for this purpose and enhanced H_2 sensing properties have been achieved [14]. Even though hydrogen is the simplest element, it is an unavoidable impurity during synthesis and easily adsorbed on the nanowire surface, and it is known to influence the doping characteristics of GaN significantly [15].

Existing density functional theory (DFT) studies on the H_2 sensing properties of GaN nanowires have focused mainly on aspects such as the stability of H_2 at the surface. The enhanced gas sensing properties in presence of metals has been investigated [11,12]. Nevertheless, which alkali metal is superior in performance when it comes to H_2 sensing is not yet ascertained in detail. Pt and Pd are known to be two superior elements when it comes to H_2 gas sensing. In this report, we are investigating the H_2 sensing properties of Pt and Pd functionalized GaN nanowires and compare their properties. We focus on the energetics, and electronic structure changes brought about by the presence of metal functionalization as well as H_2 adsorption. Since the surface energies of GaN

nanowires grown along [0001] direction is reported to be lower than other orientations [16,17], we are focusing on wurtzite GaN nanowires in the [0001] orientation in the present investigation.

Computational methodology

A wurtzite $Ga_{48}N_{48}$ nanowire with [0001] orientation, having a hexagonal cross section and a diameter of 9.6 Å is modeled and subjected to optimization (see, figure 1.a). The length of the nanowire supercell along Z direction is 10.5 Å. To make the interaction between the periodic images negligible, a vacuum region of 25 Å is added along the X and Y directions and periodic boundary conditions are applied along the Z direction. The nanowire thus presents a hexagonal cross section as shown in figure 1.a, with six side faces of the (100) crystal plane.

The plane wave pseudo potential code, *Vienna Abintio Simulation Package* (VASP) is used to carry out the DFT simulations [18]. The interaction between the ionic core and valence electrons are treated using the projector augmented wave (PAW) method [19,20]. The exchange and correlation interactions are described by the generalized gradient approximation (GGA) in the Perdew Burke Ernzerhof (PBE) formalism [21,22]. To account for the strong electronic correlations existing in GaN, the Hubbard parameter is included for Ga, with the following values, U=6.7eV and J =0.7 eV, in the Dudarev's method, as implemented in VASP. These values were previously used in studies that could successfully reproduce experimental results [3,23]. Kinetic energy cut off of 550 eV is used to expand the plane waves included in the basis set, which is previously shown to be sufficient for GaN with PAW-PBE pseudo potentials [24,25]. The convergence of k-grid with respect to the supercell size has been examined and for the Brillouin zone integration, a Gamma centered k-grid of 1x1x8 is employed. Energy and force tolerances of 10^{-6} eV and 0.001 eV/Å, are adopted for the relaxation of atomic coordinates to ensure necessary accuracy. Extant literature has shown that the inclusion of vander Waals interactions didn't alter the geometries and band structures of the H_2 and metal functionalized GaN nanowires compared to the PBE level calculations. Hence in the present study, we haven't included these corrections [26].

Results and discussion

The pristine GaN nanowire in the [0001] orientation is subjected to optimization and the relaxed structure is shown in figures 1.a and 1.b. The Ga-N bond lengths in the optimized geometry vary between 1.98 to 2.08 Å. This relaxed geometry is used to carry out the adsorption energy calculations, and to find the most probable adsorption sites for Pd and Pt atoms on the GaN surface, we have taken different configurations into consideration. We investigate in total 6 positions, that include bridge, center and two positions each on top of Ga and N atom as indicated in figure 1.b. The bridge position is in the middle point of a Ga-N bond, while the center position is in the center of the hexagonally coordinated atomic ring. The adsorption energies for Pd and Pt are calculated by the formula,

$$E_{ads} = E_{GaN:M} - E_{GaN} - \mu_M \qquad (1)$$

The adsorption energy with H or H_2 adsorption is calculated as,

$$E_{ads\ (H/H2)} = E_{GaN:M+H/H2} - E_{GaN:M} - \mu_{H/H2} \qquad (2)$$

where $E_{ads\ and}$ $E_{ads\ (H/H2)}$ is the adsorption energy in respective cases. The first and second term on the right-hand side (RHS) of equation (1) denote the total energy of the nanowire after and before adsorption of Pd/Pt. In equation (2), the first and second terms on the RHS represent total energy of the nanowire after and before adsorption of hydrogen. The last term on the RHS denotes the chemical potential (μ) of the metal atom, corresponding to atomic hydrogen or hydrogen molecule depending on the adsorbate. For pristine GaN nanowire with hydrogen molecule adsorbed on it, the chemical potential of hydrogen molecule (-6.76 eV) is used for the calculations, while for GaN-Pd/Pt nanowires the chemical potential of atomic hydrogen (-0.028 eV) is used. This is because the hydrogen molecule dissociates and attach as H atoms in presence of Pd/Pt atoms. The chemical potential of Ga is calculated as the energy of a Ga atom in bulk gallium, assuming Ga rich conditions. Hence under thermodynamic equilibrium, that of N is calculated from, $\mu_{Ga} + \mu_N = \mu_{GaN}$ where μ_{GaN} is the chemical potential of bulk GaN. The chemical potential of Pd and Pt is calculated as the energy of a single atom. The values of chemical potentials thus calculated are, Ga=-3.07 eV,

N= -9.09 eV, Pd= -1.47eV and Pt = -0.56 eV. The calculated adsorption energy values are shown in table 1.

The negative adsorption energies indicate that adsorption of Pd and Pt are exothermal, and the adsorption sites are stable. Only for the bridge position for Pt, a positive adsorption energy is obtained, indicating that this site is energetically less favorable than the others. Pt is slightly more stable than Pd, as seen from the more negative energy values. We also study the adsorption of a H_2 molecule on the pristine GaN nanowire, and further compare it with the most stable metal functionalized nanowire. Since the Ga1 position is the most stable adsorption site for both Pt and Pd atom, from the lower adsorption energies, for further calculations, this configuration is considered. We study two different cases such as hydrogen adsorbed on (a) pristine and (b) Pt/Pd functionalized nanowire. It can be seen that in the pristine nanowire also, H_2 adsorption can happen under favorable circumstances, as evident from the negative adsorption energies. In the presence of Pd and Pt, the metal atoms act as a connection link to attach hydrogen as it gets attached to the nanowire through the bonding through metal atoms. The top view and side view of the H_2 attached on the metal functionalized nanowire is shown in figures 1.b and c respectively. It is interesting to see that H_2 dissociates and attached as two separate atoms to the metal atom, which has also been observed in previous studies [13,14]. Figures 1(c) and 1(d) shows H_2 attach to the pristine GaN nanowire and hydrogen atom attached through the Pd/Pt atoms to the GaN nanowire respectively.

The bond lengths of the different atoms in the nanowire after adsorption is shown in table 2. The Ga-N bond lengths in the optimized pristine nanowire vary between 1.8 to 2 Å. The average Ga-N intra layer bond lengths are 2.0 Å while the inter layer bond distance is 1.87Å. The shortest intra layer bond lengths are obtained for the center layers, while towards the surface, the bonds are more extended. When H_2 is adsorbed on the pristine nanowire, the bond length of the molecule after structural optimization is 0.75 Å, and the distances of the Ga and N atoms in the near vicinity is 4.4 Å and 3.52 Å respectively. The bond lengths of Pd and Pt adsorbed nanowires are calculated for the most stable geometry and shown in table 2. The Ga-N bond lengths are consistent, and the

Pd atom is attached to the most stable top position, with bond distances of 2.33Å and 2.05Å from the Ga and N atoms respectively. When hydrogen is attached to the nanowire through this Pd atom, it prefers to stabilize as two separate H atoms at a Pd-H bond distance of 1.66 Å. The H-H bond distance is 0.89 Å, larger than the bond length of hydrogen molecule. The Pd atom's distance to Ga and N atoms slightly adjusts after H adsorption. In the case of Pt, the H-Pt bond distances are further reduced to 1.57 Å, and the H-H distance is 1.25 Å. In both the above situations, in presence of Pd and Pt, the H molecule dissociates and chemically adsorbed to the transition metal atom. It is observed that when hydrogen is adsorbed, the nearest neighbor Ga-N bond lengths change, as can be seen from table 2. For both Pd and Pt adsorbed nanowires, the Ga-N bond lengths after optimization are 1.93Å to 2.03Å, after the attachment of hydrogen. This change in bond lengths can manifest as a strain in the nanowire surface and can be used as a parameter to understand the hydrogen detection.

We perform electronic structure calculations to understand the H_2 sensing mechanism in more detail. The total density of states (TDOS) calculated for the pristine as well as Pt/Pd adsorbed nanowires are shown in figure 2. From the TDOS plots it can be seen that with Pd and Pt adsorption, the conduction band minimum is lowered and narrowing the band gap. Further, an additional peak appears near the conduction band minimum, arising due to the hybridization and coupling owing to the metal addition. To understand this in detail, and to figure out the contribution of various atomic orbitals, we have plotted the partial density of states (PDOS) of the above systems. We show the PDOS from -2 to 2 eV. The PDOS shows that the Ga *p* and N *p* states show significant changes around the valence band maximum, owing to the interaction with the adsorbed metal atoms. The valence band maximum is mainly constituted by the *d* and *s* orbitals of Pt and Pd. The conduction band moves to the lower energy side for both Pd and Pt doped nanowires, due to the hybridization and coupling of the host Ga and N atomic orbitals with that of Pt and Pd. This change in electronic properties of the nanowires with hydrogen adsorption can help to understand the detection mechanism of the GaN nanowire.

Further, the bader charge analysis is carried out to estimate the charge transfer and presented in table 3. The charge acquired by the N atom changes with hydrogen attachment, in the Pt and Pd adsorbed nanowire. The variation in charge of transition metal atoms with H attachment show that, the Pt/Pd-H bond is more of ionic character. It is seen that the more electronegative N gains and Ga loses charge. Though Pd and Pt has the same electro negativity, Pt gains more charge than Pd. This is owing to the slight reduction in charge gain of N atom in the vicinity of Pt. For the pristine GaN nanowire, hydrogen retains the molecular bond characteristics by sharing charge. When H is adsorbed on to the nanowire, through the metallic atom, it dissociates into two H atoms and acquires small negative charge. Interestingly the charge depreciation of Ga atoms remains consistent with metal atom and H_2 adsorption. For N, it varies from 3.07 e^- for the pristine nanowire to 2.54 e^- for the nanowire with Pt adsorption and slightly increases to 2.72 e^- with hydrogen attachment. This charge accumulation/depletion with adsorption of metal atoms and hydrogen can be used as an entity to understand the hydrogen detection.

Furthermore, the difference in charge density between GaN-Pd/Pt nanowire with and without hydrogen adsorption is plotted to understand the charge reconstruction happening at the surface. The charge density difference plot is presented in figure 3. It is seen that when hydrogen atoms are attached to the Pd and Pt atoms after dissociation, there occurs a charge redistribution in the surrounding atoms. The charge gain of both Pd and Pt atoms reduces as indicated by the large yellow regions surrounding the Pd-H and Pt-H bonds. Moreover, since the charge is largely concentrated on the atoms, than towards the middle of the bond, both Pd-H and Pt-H bonds possess more ionic character. It can also be seen that the N atoms in the near vicinity of the Pd/Pt atoms lose charge as shown by the large yellow regions surrounding them. Moreover, the charge reconstruction is enhanced for the Pt adsorbed nanowire upon hydrogen adsorption. Hence Pt is a more efficient transition metal that can be used to tune the surface adsorption properties of GaN nanowire and can aid in hydrogen sensing.

Conclusions

We have systematically studied the adsorption mechanism of Pd and Pt on GaN nanowires oriented along the [0001] direction and further analyzed the hydrogen sensing properties. From the 6 different adsorption sites considered, the position on top of a Ga atoms is the most stable one energetically. The attachment of hydrogen causes a strain, that manifest as change in adjacent Ga-N bond lengths and the bader charge analysis show change in electronegativity of N atoms in the Pd/Pt adsorbed nanowires. The calculations have shown that Pt atom adsorbed on a top site over Ga atom possess the lowest adsorption energy. Further, hydrogen dissociates to attach as atoms to this site, and induces reduction in band gap, which combined with increased charge gain makes it the most efficient for hydrogen sensing. To conclude, the change in surface potential induced by the hydrogen attachment to the Pt site, as well as the lattice strain indicates that the hydrogen sensing performance of GaN nanowires can be enhanced by Pt adsorption.

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Table 1. The adsorption energies of GaN nanowires with Pt and Pd and H_2 adsorption. The last column presents the adsorption energy of pristine GaN nanowire with H_2 adsorption

Adsorption sites		Ga1	Ga2	N1	N2	Bridge	Centre	(GaN-Pd/Pt+H_2)	Pristine GaN + H_2
Adsorption energy (eV)	Pt	-3.61	-3.37	-3.28	-2.84	0.55	-1.76	-8.55	-0.02
	Pd	-2.38	-1.91	-2.14	-2.05	-0.55	-1.9	-7.93	

Table 2. The bond lengths (in Å) of the pristine as well as Pd and Pt functionalized nanowire with and without H_2 adsorption

Bond lengths (Å)											
Pristine		Pristine + H_2		Pd-GaN		Pd-GaN+ H_2		Pt-GaN		Pt-GaN + H_2	
Ga-N	1.89	Ga-N	1.89	Ga-N	1.94 2.0	Ga-N	2.03 1.94	Ga-N	1.97	Ga-N	1.93 1.96 2.03
		Ga-H	2.68	Ga-Pd	2.53	Ga-Pd	2.53	Ga-Pt	2.53	Ga-Pt	3.14
		N-H	2.96	N-Pd	2.05	N-Pd	2.10	N-Pt	1.96	N-Pt	2.08
		H-H	0.75			Pd-H	1.66			Pt-H	1.57
						H-H	0.89			H-H	1.25

Table 3. Bader charge analysis of GaN nanowires with adsorbates. The Ga and N atoms are the ones either directly bonded or in the near vicinity of the adsorbates

Nanowire configuration	Charge			
	Ga	N	Pd/Pt	H
GaN+Pt	3	−2.54	−0.56	
GaN+Pd	3	−3.02	−0.41	
GaN+H_2	3	−3.07		0.01 −0.01
GaN+Pd+H_2	3	−2.78	-0.39	-0.003 -0.01
GaN+Pt+H_2	2.99	−2.72	−0.37	−0.01 −0.01

Figure 1. (a) The optimized structure of GaN nanowire (b) The side view of the nanowire with different adsorption sites, where B and C represents the bridge and center respectively. Ga1, Ga2, N1 and N2 indicates the sites on top of the respective atoms. (c) The side view of pristine GaN nanowire with the H_2 molecule adsorbed (d) Side view of GaN nanowire with Pd/Pt atom, situated on the most stable adsorption site with H atoms attached to it. The purple and silver colored atoms represent Ga and N respectively

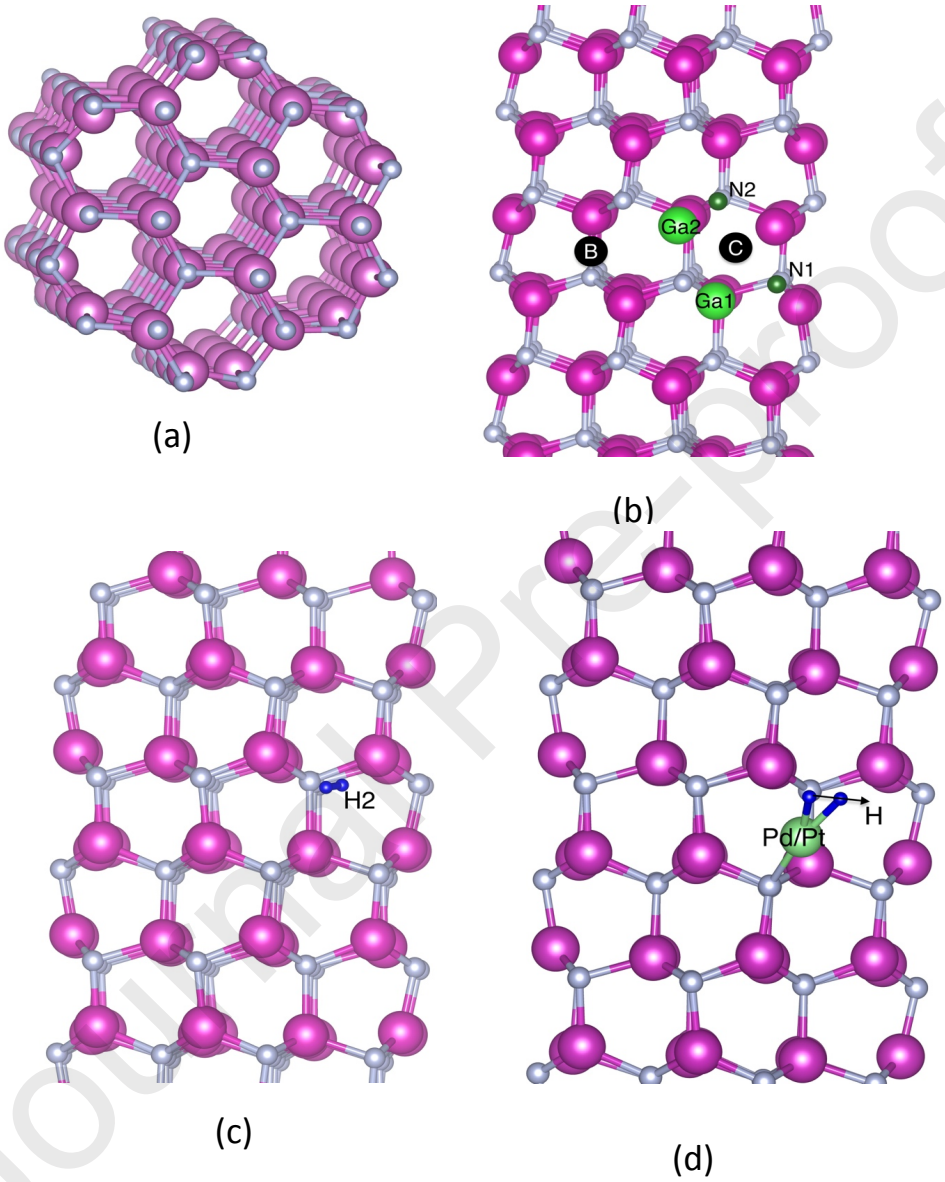


Figure 2. The Density of states of pristine nanowire as well as nanowires with Pt, Pd and hydrogen adsorption, calculated using the GGA+*U* method

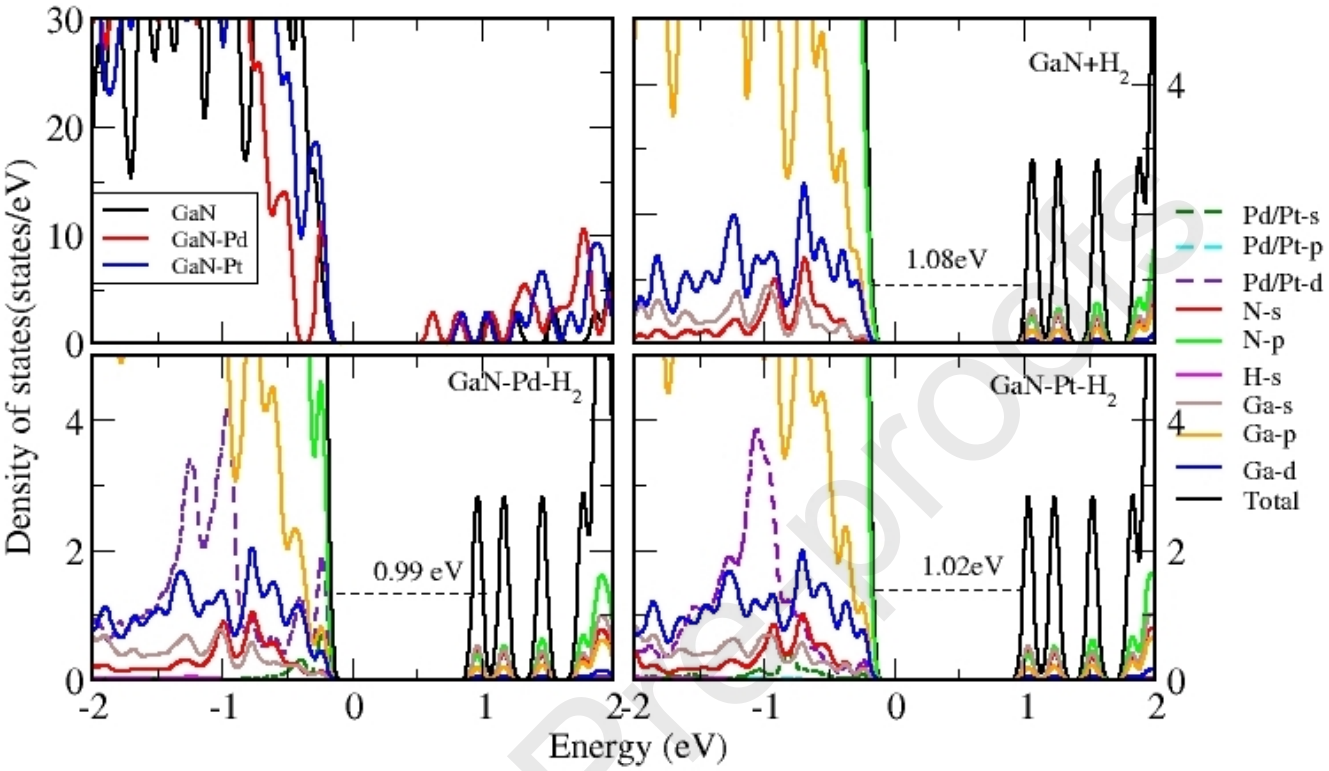
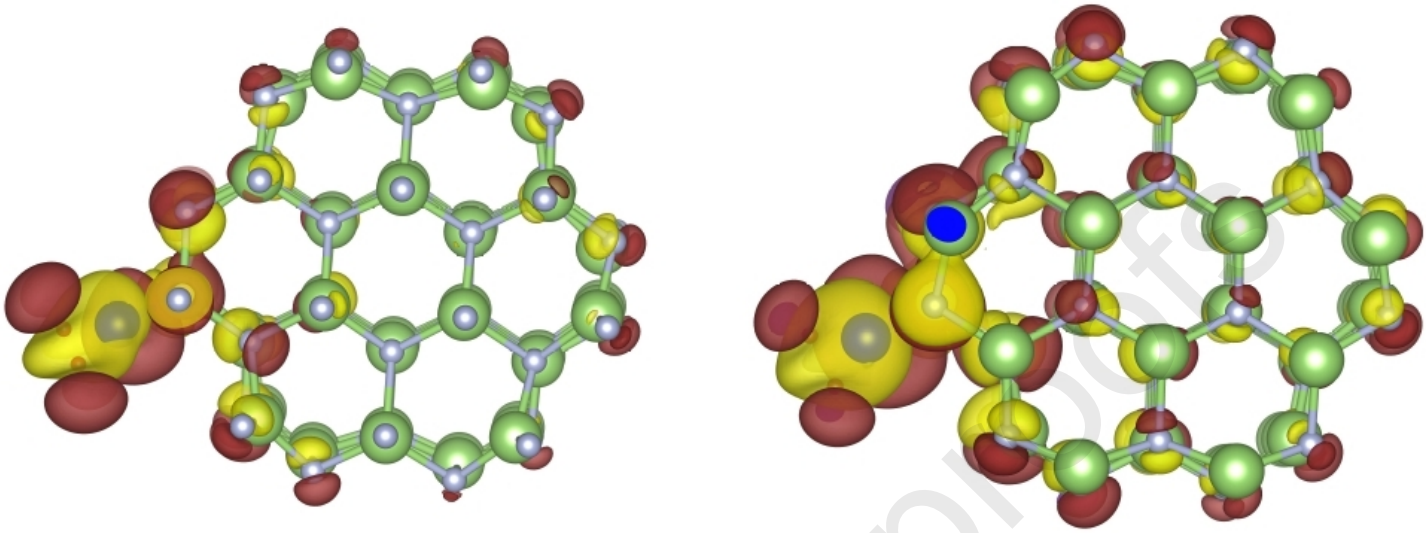


Figure 3. The charge density difference of GaN nanowire with Pd (a) as well as Pt (b) with and without hydrogen adsorption. The yellow and red regions represent charge depletion (positive) and accumulation (negative) respectively. The isosurface level is 0.01371 and the unit of charge density is $e^-/bohr^3$. The green, grey and red atoms indicate Ga, N and H respectively. The blue atom is Pd or Pt



Highlights

1. GaN [0001] nanowire is modelled using density functional theory

2. Most stable adsorbing sites for Pd and Pt adsorbates are identified

3. In the bare nanowire hydrogen attach as a molecule, while it dissociates into atoms, in presence of Pd and Pt metal functionalization

4. A change in bond-length, that can manifest as a strain on the surface as well as charge reconstruction owing to hydrogen adsorption can be utilized as entities to detect hydrogen

5. The Pt and Pd bond with H is more of ionic nature, and Pt-H bond is more compact. The lowest adsorption energy, combined with lattice strain and charge reconstruction renders Pt more efficient metal adsorbate to the GaN nanowire surface

Declaration of interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

☐The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Credit author statement

S. Assa Aravindh: Conceptualization, Methodology, Software, Writing-Reviewing and editing

Wei Cao: Validation and editing

Matti Alatalo: Editing, supervision

Marko Huttula: Editing, supervision