Piezoelectric Effects in Surface-Engineered Two-Dimensional Group **III** Nitrides

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Supporting Information

ABSTRACT: Piezoelectric effects of two-dimensional (2D) group III-V compounds have received considered attention in recent years because of their wide applications in semiconductor devices. However, they face a problem that only metastable or unstable structures are noncentrosymmetric with piezoelectricity, thus leading to the difficulty in experimental observation. Motivated by the recent advances in the synthesis of 2D group III nitrides, in this paper, for the first time, we study the piezoelectric properties of the 2D group III nitrides (XN, X = Al, Ga, and In) with buckled hexagonal configurations by surface passivation, which are thermodynamically stable. Unlike the previously reported planar graphitic structure, we demonstrate that the hydrogenated 2D nitrides (H–XN–H, X = Al, Ga, and In) exhibit both the in-



plane and out-of-plane piezoelectric effects in their monolayer and multilayer structures under an external strain in the basal plane. We further elucidate the underlying mechanism of the piezoelectricity by analyzing the correlations between the piezoelectric coefficients and their structural, electronic, and chemical properties. In addition, we show that H-F cofunctionalization not only enhances the stability, but also significantly improves the ionic polarization because of the charge redistribution, thus leading to large in-plane piezoelectric coefficients in F-XN-H. Our study advances the research in 2D piezoelectric materials and would stimulate more theoretical and experimental efforts in developing effective piezoelectric materials for device applications.

KEYWORDS: 2D group III nitrides, surface engineering, buckled structure, piezoelectricity, density functional theory

1. INTRODUCTION

Two-dimensional (2D) materials can exhibit very different properties from those of their 3D counterparts. Piezoelectricity is one of such properties because many materials that are not piezoelectric in their bulk form become piezoelectric when thinned down to monolayers.^{1,2} For example, 2D MoS₂ is first experimentally demonstrated as a piezoelectric sheet.^{3,4} The reduction in dimensionality eliminates the inversion symmetry of bulk MoS₂, so that the in-plane polarization can be induced under the external strain. Normally, materials with piezoelectricity are supposed to be structurally noncentrosymmetric and nonmetallic.⁵ In recent years, several kinds of 2D structures have been theoretically proved to possess an intrinsic piezoelectric effect, including h-BN,^{2,6¹} transitionmetal dichalcogenides (TMD),^{1,2} transition-metal dioxides,⁵ group II–VI compounds,^{2,7,8} group III–V compounds (beyond borides),^{2,9} group III-monochalcogenides,^{10,11} group IV monochalcogenides,¹² and group III₂-VI₃ compounds.^{13,14} However, it is very challenging to experimentally characterize piezoelectricity when the materials cannot exist in the 2D form. Thus, the phase stability is an additional crucial factor for 2D materials.⁵ Given this reason, we noticed that 2D group III-V compounds have such a problem in previous work.^{2,5} Although

the piezoelectric coefficients of 2D group III-V semiconductors have been already reported, most of the studied systems have a buckled hexagonal geometrical configuration, which are energetically metastable or unstable.² In fact, except for group III nitride monolayers, the ground-state structure of all the other group III-V compounds is in the buckled tetragonal phase, which has a lower formation energy than that of the buckled hexagonal one.^{15,16} Nevertheless, the tetragonal phase is centrosymmetric, and thus the piezoelectricity is suppressed by the inversion symmetry. For group III nitrides, the planar graphitic structure was considered to be stable with the in-plane piezoelectricity.^{2,17,18} However, unlike graphene, most N p_z electrons are quite localized, forming the nonbonding orbitals,¹⁹ so it is difficult to efficiently stabilize such a structure because of the high surface energy. Therefore, the piezoelectric effects of the theoretically studied planar group III nitrides might not be observed in experiments.

Recently, 2D GaN sheet has been successfully synthesized via a migration-enhanced encapsulated growth technique and



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nitrification reaction, respectively.^{20,21} More importantly, it was demonstrated that the structural buckling leads to the thermodynamically most stable structure for 2D group III nitrides, which can be achieved by using hydrogen to passivate the unsaturated states.²² Compared with the planar configuration, the buckled phase possesses a Janus structure with the nonequivalent surfaces. Therefore, it not only lacks the inversion center, but also breaks the mirror symmetry in the vertical direction, and hence can exhibit both the in-plane and out-of-plane piezoelectricity.

In this paper, we report a theoretical study on the piezoelectric effects of group III nitrides (XN, X = Al, Ga, and In) buckled monolayers and multilayers by using first-principles calculations. We determine the piezoelectric coefficients to evaluate their performance in nanoscale electronic and energy applications. In addition, we explore the underlying mechanism of the piezoelectric effect in these materials, that is, the correlation between piezoelectric coefficients and their structural, electronic, or chemical properties. Finally, we propose that hydrofluorination can further enhance the piezoelectric performance of the 2D group III nitrides.

2. COMPUTATIONAL METHODS

First-principles calculations based on density functional theory are carried out for the studied systems. The electronic exchangecorrelation interaction is treated using the Perdew-Burke-Ernzerhof functional within generalized gradient approximation.²³ The all-electron projector-augmented wave method^{24,25} implemented in the Vienna Ab initio Simulation Package (VASP)²⁶ is applied to study the ground-state structure and electronic properties. The energy cutoff is set at 500 eV. The convergence criteria for energy and force are set as 0.0001 and 0.01 eV/Å, respectively. The Brillouin zone is represented with $15 \times 15 \times 1$ Monkhorst-Pack special k-point meshes for the hexagonal lattice when optimizing the structure and with $15 \times 23 \times 1$ k-point meshes for the rectangle lattice when calculating the piezoelectric and elastic stiffness coefficients.²⁷ A vacuum space of 20 Å in the direction perpendicular to the sheet is used, which is sufficient to avoid interactions between two neighboring layers. The elastic stiffness coefficients are calculated using the finite difference methods,²⁸ and the coefficients of the piezoelectric tensor e_{ij} are obtained by using both the density functional perturbation theory and the Berry phase method³¹ as implemented in VASP. The description of piezoelectric tensors can be found in the Supporting Information.

3. RESULTS AND DISCUSSION

In the planar graphitic structure of group III nitrides as shown Figure 1a, N atoms are sp²-hybridized. Only a small part of the p_z electrons form π bonds with the nearby X (X = Al, Ga, and In) atoms; therefore, the top of the valence band (see Figure S1 in the Supporting Information) is mainly composed of the nonbonding p_z orbitals, leading to a more chemically active surface with less stability compared to graphene.¹⁹ A possible way to enhance the stability is using hydrogen to passivate the unsaturated states (Figure 1b), which has been investigated by recent studies.^{20,22} Binding energy calculations (see Figure S2 in Supporting Information) clearly show that hydrogenpassivated structures are more stable than those without the passivation. The hydrogenation on the top site of N and X atoms distorts the planar geometry, resulting in a small buckling within the basal plane. The difference in bonding between H-X and H-N gives rise to nonequivalent charge distribution. For example, Figure 1c shows the charge density distribution of the buckled AlN sheet, where more charges are

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Figure 1. Crystal structures of the (a) planar and (b) buckled group III nitrides. The buckled configuration is thermodynamically most stable. (c,d) Charge density distribution and electrostatic potential file of the H–AlN–H sheet, respectively. The green dashed line connects the two H atom minima on the electrostatic potential curve.

concentrated around N atoms. This imbalance breaks the mirror symmetry along the vertical direction in the planar structure, thus the two surfaces of the buckled AlN are anisotropic, which can also be demonstrated from the energy step $(\Delta \phi)$ in its electrostatic potential file (see Figure 1d, marked by black dashed lines). Because of these characters in such Janus configuration, we first study the piezoelectric properties of the monolayer buckled group III nitrides by applying a uniaxial strain along the armchair direction (strain along the zigzag direction would give the same results because of the 3*m* symmetry of the studied structures). Although the planar phase is not the most stable, it is still useful to compare it with our results; thus, we summarize the data of both structures in Table 1.

For convenient discussion, we use H-XN-H (X = Al, Ga, and In) to denote the hydrogenated 2D group III nitride sheets. From Table 1, one can see that the values of both e_{11} and d_{11} piezoelectric coefficients in the H–XN–H monolayer are smaller than those in the corresponding planar XN. A rational understanding is that the polarization of XN is confined within the basal plane without any component in the vertical direction. However, because of the structural buckling in H-XN-H, the contribution to piezoelectricity from the polarized X-N bonds is divided into two directions, which causes a weaker in-plane piezoelectric effect. We can also infer the trend from Table 1 that e_{11} becomes larger from Ga (0.35 $\times 10^{-10}$ C/m) to In (0.40 $\times 10^{-10}$ C/m) to Al (0.65 $\times 10^{-10}$ C/m), which is different from that in TMD (MX₂, M = Mo and W; Y = S, Se, and Te), where the heavier chalcogenide leads to a larger e_{11} value.^{1,2,32} Here, we find that e_{11} of H– XN-H has a good linear relationship with the electronegativity difference $(\Delta \chi)$ of the group III elements and nitrogen (see Figure 2a), where $\Delta \chi$ values for Al–N, Ga–N, and In–N are taken to be 1.43, 1.23, and 1.26, respectively. This is understandable as a lager $\Delta \chi$ can increase the noncoincidence degree of the centers of positive and negative charges when the structure is externally strained, which is the origin of the piezoelectricity. For d_{11} , the magnitudes listed in Table 1 are 1.15, 0.63, and 1.35 pm/V for H-AlN-H, H-GaN-H, and H-InN-H, respectively. The largest value occurs in H-InN-H rather than H–AlN–H because the difference between C_{11} and C_{12} in H-InN-H is only half of it in H-AlN-H. For mechanical properties, we find that the elastic modulus of H-XN-H is mainly determined by their bond length because of the structural similarity among these three monolayers. Figure

		e ₁₁	e ₃₁	C ₁₁	C ₁₂	d_{11}	<i>d</i> ₃₁
AlN	planar ^b	2.23		148.10	67.10	2.75	
	planar	2.28		144.75	66.37	2.90	
H–AlN–H	1-layer	0.65	0.44	85.50	28.86	1.15	0.39
	2-layer ^Z	1.43	0.54	170.14	56.58	1.26	0.24
	3-layer ^Z	2.31	0.69	254.80	85.28	1.37	0.20
	2-layer ^W	1.57	0.62	173.09	54.62	1.32	0.27
	3-layer ^W	0.54	0.66	258.70	79.80	0.31	0.19
GaN	planar ^b	1.48		141.70	67.9	2.00	
	planar	1.49		136.81	65.56	2.09	
H-GaN-H	1-layer	0.35	0.30	78.60	25.32	0.63	0.29
	2-layer ^Z	1.01	0.44	149.82	53.26	1.05	0.22
	3-layer ^Z	1.55	0.49	213.61	82.71	1.19	0.16
	2-layer ^W	0.60	0.44	152.41	51.66	0.60	0.22
	3-layer ^W	0.49	0.55	225.94	77.21	0.33	0.18
InN	planar ^b	2.24		98.40	57.70	5.50	
	planar	2.26		94.04	55.52	5.87	
H–InN–H	1-layer	0.40	0.39	52.55	22.94	1.36	0.51
	2-layer ^Z	1.04	0.51	99.57	43.54	1.86	0.36
	3-layer ^Z	1.89	0.61	144.44	67.41	2.45	0.29
	2-layer ^W	1.04	0.54	100.00	44.61	1.86	0.37
	3-layer ^W	0.9	0.63	147.60	62.43	1.05	0.30
F-AlN-H	1-layer	8.85	0.42	89.00	34.72	16.30	0.34
F-GaN-H	1-layer	6.12	0.49	73.99	35.06	15.72	0.45
F–InN–H	1-laver	2.42	0.33	54.96	28.12	9.02	0.40

Table 1. Piezoelectric and Mechanical Properties of the Surface-Engineered 2D Group III Nitrides^a

^{*a*}The values of planar configuration in the previous study are also given here for comparison. Elastic coefficient in units of N/m, piezoelectric coefficients e_{11} in 10⁻¹⁰ C/m and d_{11} in pm/V. ^{*b*}Data are from ref 2. Our results are in good agreement with ref 2. The superscripts Z and W represent the stacking sequence along zinc blende (111) and wurtzite (0001) directions in multilayer H–XN–H, respectively (see Figure 3).



Figure 2. (a) Correlation between the piezoelectric coefficient of group III nitride (H-XN-H, X = Al, Ga, and In) buckled monolayer and the corresponding electronegativity difference. (b) Correlation between the elastic stiffness coefficient and the bond length in H-XN-H.

2b shows a positive and almost linear correlation between elastic stiffness coefficients and the reciprocal of the X–N bond length, which clearly demonstrates the inverse proportional relationship between them. Therefore, because of the larger radius of the In atom, deformation can more easily happen under the external strain in the H–InN–H sheet. In addition, compared with the planar XN, we note that C_{11} and C_{12} become smaller in the buckled phases (see Table 1). The reason for the reduction of elastic stiffness is that hydrogen passivation breaks the sp² hybridization of N atoms; thus the π cloud, which can enhance the mechanical strength, disappears.²⁰ Similar behaviors have been also observed in the hydrogen saturated graphene.³³

In addition to the in-plane piezoelectricity, it is more important to see that the H-XN-H (X = Al, Ga, and In) monolayers also possess the vertical polarization, which is missing in the planar structure. Although the out-of-plane piezoelectric properties in some other group III-V compounds were reported in previous studies,² it is still unclear whether these metastable 2D structures can be realized in the future. Thus, the synthesized H-XN-H is most likely to be confirmed with vertical piezoelectric effects in the experiment. According to our calculations (the details are given in Figure S3 in Supporting Information), the values of e_{31} for H–AlN– H, H–GaN–H, and H–InN–H are 0.44 \times 10 $^{-10}$, 0.30 \times 10^{-10} , and 0.39×10^{-10} C/m, respectively. We also note that e_{31} is positively related to the electronegativity difference $(\Delta \chi)$ between the element X and N, but it does not show the linear relationship (see Figure 2). The possible reason is that apart from the X-N bonds, the H-N bonds parallel to the z-axis also contribute to the vertical polarization, and the polarized direction of these two bonds is opposite, so the coupling between them may destroy the linear correlation. By considering the elastic stiffness, we then obtain the values of d_{31} in H–XN–H monolayers. Similarly, H–In–H has the largest value (0.51 pm/V) among these three structures, which is benefitted from the smaller sum of C_{11} and C_{12} . Compared with the recent discovered Janus TMDs (MXY, M = Mo and W; X, Y = S, Se, and Te),³² both e_{31} and d_{31} of H–XN–H are about 1 order of magnitude larger than the values in these monolayer materials, which exhibits potentials in flexible fabrication of the piezoelectric devices.

Next, we study the piezoelectric effect in the hydrogenated group III nitride multilayers for two reasons: (1) the buckled structure is the preferred configuration, regardless of the number of layers;²⁰ (2) additive effect may enhance the piezoelectric performance in multilayer structures. There are two possible ways to cleave a multilayer structure from the bulk phases of group III nitrides, that is, along the (111) surface of the zinc blende phase (Z-type) and along the (0001) surface of the wurtzite phase (W-type) (see Figure 3). Total



Figure 3. Geometrical structures of (a) Z-type and (b) W-type group III nitride bulk, 2-layer, and 3-layer sheets.

energy calculations show that the Z-type is more stable than the W-type, but the energy difference is very small ($\sim 0.05 \text{ eV}/$ cell); therefore, we consider these two configurations to be energetically degenerate. We first investigate the piezoelectric effect in Z-type multilayers. We find that the in-plane piezoelectric coefficients e_{11} and d_{11} increase with the thickness of layers (see Table 1). To understand the reason, we analyze the geometrical structures of the bilayer and trilayer sheets. As shown in Figure 3a, the two layers are parallel stacked (ABCABC...) without the inversion center; therefore, the piezoelectric polarization remains rather than canceling each other out. Moreover, the two adjacent layers are chemically bonded, so that the external strain can be transferred from one layer to the other, leading to a strong coupling between them. This is different from the layered Janus TMDs, where the interface interaction is the van der Waals (vdW) force, which is too weak to form effective coupling and hence has little effect on the in-plane piezoelectricity.³² From Figure 4a-c, we find that, like monolayer, the trends for e_{11} and d_{11} of bilayer and trilayer are not same either because of the variability of C. In this case, the mechanical stiffness destroys the positive relationship to the electronegativity difference $(\Delta \chi)$ and has an obvious effect on the value of d_{11} . Among these three systems, we observe that the smaller C_{11} (Figure 4b) of H-InN-H induces a much larger d_{11} coefficient (Figure 4c), especially in its trilayer structure (2.45 pm/V), which is comparable to that of the α -quartz (2.3 pm/V),³⁴ implying the potential of the in-plane piezoelectric effects in this structure. Importantly, it is worth to note that the bulk zinc blende phase has a cubic lattice (Figure 3a) with the space group of no. 216; therefore, all the piezoelectric coefficients are suppressed by its structural symmetry ($F\overline{4}3m$). This indicates that e_{11} and d_{11} will disappear, when the slab becomes thick enough showing the characters of the bulk phase, and the correlation plotted in Figure 4 may only explain the piezoelectric behavior of the ultrathin film.



Figure 4. Variation trend of (a) e_{11} , (b) elastic stiffness coefficients, (c) d_{11} , and (d) e_{31} of the Z-type group III nitride multilayers with respect to the thickness. (e) Electrostatic potentials of the H–In–H monolayer, bilayer, and trilayer. Dashed lines connect the H atom minima on each curve. (f) Correlation between d_{31} and inherent electric field of the Z-type group III nitride slabs.

For the out-of-plane piezoelectric effect, e_{31} also increases as the number of layers becomes higher (see Figure 4d), while d_{31} exhibits a decreasing trend because the elastic stiffness increases more quickly (see Figure 4b). Here, we use the inherent electric field to evaluate the vertical piezoelectricity, which is induced by the opposing X- (X = AI, Ga, and In) and N-terminated surfaces. The magnitude of the electric field perpendicular to the 2D layer can be determined by the slope of the plane-averaged electrostatic potential between the H atom minima,²² as plotted in Figure 1d. For instance, the calculated values of the electric field are 0.42, 0.37, and 0.33 eV/Å for 1-layer, 2-layer, and 3-layer hydrogenated InN sheets, respectively (Figure 4e). This shows that the electric field becomes weaker in a thicker slab. The reduction in electric field strength results from the existence of opposing polarized In-N bonds in multilayer structures as shown in Figure 3a, where the In-N bonds in the basal layers and those between two adjacent layers are polarized in an opposite way, so that the polarization is partially canceled by each other. From Figure 4f, one can see that there is an almost linear correlation between d_{31} and the inherent electric field in H–InN–H, and such a relationship is also suitable for H-AlN-H and H-GaN-H systems, implying that the strength of vertical polarization has a significant impact on the out-of-plane piezoelectricity, and the monolayer structures are notable candidates with the higher d_{31} coefficients. Here, we should also note that once the number of layer becomes larger, the d_{31} coefficients will be suppressed because the inherent electric field induced by the nonequivalent surface disappears under the symmetry protection.

For W-type multilayer structures, we do not observe a monotonic relationship for e_{11} and d_{11} with respect to the number of layers (see Table 1). An intuitive way to understand it is, compared with the Z-type configuration, two adjacent layers are antiparallelly bonded in the ABAB stacking order (Figure 3b); thus, the in-plane piezoelectric effect is partially canceled. However, the values of e_{31} and d_{31} exhibit almost the same trend with that of Z-type (see Table 1), implying the outof-plane piezoelectricity relies little on the stacking sequence. Note that the bulk wurtzite phase has a lower symmetry than that of zinc blende. The $P6_3mc$ symmetry allows the polarization along the (0001) direction (Figure 3b);^{35,36} therefore, e_{31} and d_{31} can be still remained under the inplane strain in a thicker film. To check the effect of vdW force on the piezoelectric properties in multilayered 2D group III nitrides, we repeat the calculation by adding the vdW corrections (see Table S1 in Supporting Information). Both methods give nearly the same results, implying that vdW correction has a subtle effect on the piezoelectricity of these multilayer structures.

Although we have already identified the piezoelectric effect in hydrogenated 2D group III nitrides, the values of both d_{11} and d_{31} coefficients still have a large room to be improved. Because all the atoms of 2D XN (X = Al, Ga, and In) belong to the surface, piezoelectricity can be effectively engineered by the surface modification. Here, we take GaN as an example to consider the piezoelectric properties in this sheet cofunctionalized with H and F atoms. Because of the different electronegativity, F atoms are attached to the Ga site, while H atoms bind on the N site (labeled as F–GaN–H, as shown in Figure 5a). To confirm the stability, we calculate the formation energy (E_f) of both hydrogenated and hydrofluorinated GaN monolayer defined as



Figure 5. Charge transfer in (a) F-GaN-H and (b) H-GaN-H monolayers. Light blue, brown, dark blue, and white spheres represent F, Ga, N, and H atoms, respectively.

$$E_{\rm f(H-GaN-H)} = E_{\rm H-GaN-H} - E_{\rm GaN} - E_{\rm H_2}$$
(1)

$$E_{\rm f(H-GaN-F)} = E_{\rm F-GaN-H} - E_{\rm GaN} - 1/2E_{\rm H_2} - 1/2E_{\rm F_2}$$
(2)

where *E* represents the total energy, and the subscripts denote the corresponding materials. The $E_{\rm f(H-GaN-F)}$ is $-3.99~\rm eV/unit$ cell, which is lower than $E_{f(H-GaN-H)}$ (-0.80 eV/unit cell), implying that F-GaN-H possesses a higher stability and hence is also experimentally feasible. In Table 1, we give the elastic and piezoelectric properties of the monolayer F-GaN-H as well as F-AlN-H and F-InN-H. For out-of-plane piezoelectricity, there are no obvious improvements for e_{31} and d_{31} coefficients of the H-F cofunctionalized monolayers, possibly because the small slab thickness inhibits the spatial separation of positive and negative charges and hence constrains the vertical polarization. On the contrary, we find that the replacement of H with F on the Ga site has a significant effect on the in-plane piezoelectricity. Both e_{11} and d_{11} in monolayer F–GaN–H are 1 order of magnitude higher than that of H-GaN-H. To understand it, we plot the charge transfer obtained from the Mulliken population analysis in Figure 5. The major difference between hydrofluorination and hydrogenation is that there are additional electrons (~ 0.43 e) moving from Ga to F atoms, which leads to a stronger electropositivity of Ga ions than the case of H-GaN-H. As we know, piezoelectricity is contributed by both electronic and ionic polarization. Although the charge transfer between Ga and N atoms remains almost unchanged (i.e., the electronic contribution varies little), the ionic contribution is significantly enhanced in this case, so that it enlarges the coefficients of e_{11} and d_{11} . The existence of F atoms does not directly contribute to the in-plane piezoelectricity, but has an important effect on the charge distribution. It is glad to see that the values of d_{11} in the F-XN-H (X = Al, Ga, and In) monolayer are higher than that of the bulk GaN (3.1 pm/V) and AlN (5.1 pm/V).³⁶ Combined with their thin film structures, these materials may have great potentials in the application of microelectromechanical systems.³⁷

4. CONCLUSIONS

Previously studied 2D group III–V compounds with piezoelectric effects have been found to be metastable or unstable, while the piezoelectricity in their ground-state structures is suppressed by the inversion symmetry. In our study, we have investigated the piezoelectric properties of the most stable 2D group III nitrides with a noncentrosymmetric buckled hexagonal configuration. We showed that the in-plane strain not only leads to a piezoelectric effect within the basal plane of the hydrogenated XN (X = Al, Ga, and In) sheet, but also induces the change of polarization in the vertical direction, showing the out-of-plane piezoelectricity, which is missing in

the reported planar graphitic configuration. We further identified the correlations for each configuration with their structural, electronic, and chemical properties, and found that e_{11} coefficient of the H-XN-H monolayer has a linear relationship with the electronegativity difference of the elements X and N, and d_{31} is correlated to the self-induced inherent electric field in multilayer structures. In addition, we demonstrated that because of the enhancement of ionic polarization induced by charge transfer between F and X atoms, the hydrofluorination of the 2D nitride surfaces significantly enhances the in-plane piezoelectric coefficients, namely, the coefficient d_{11} (9.02-16.03 pm/V) in the monolayer is larger than that of the conventional 3D piezoelectric materials such as bulk GaN (3.1 pm/V) and AlN (5.1 pm/V), suggesting that surface engineering is an effective way to modulate the piezoelectric properties. We hope that these findings can stimulate more efforts in the design and synthesis of novel 2D materials with stable geometry and super-piezoelectric performance for future device applications.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acsami.8b17341.

Description of piezoelectric tensors, band structure and density of states of the planar graphitic AlN, comparison of binding energy between 2D group III nitrides with and without hydrogen passivation, and relationship between a uniaxial in-plane strain and the change of induced polarization perpendicular to the sheet, and effect of vdW force on the piezoelectric properties in multilayered 2D group III nitrides (PDF)

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Notes

The authors declare no competing financial interest.

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