Sheng Gong,<sup>‡</sup> Cunzhi Zhang,<sup>‡</sup> Shuo Wang,<sup>‡</sup> and Qian Wang<sup>\*,†,‡</sup>

<sup>†</sup>Center for Applied Physics and Technology, College of Engineering, Peking University, Beijing 100871, China <sup>‡</sup>Department of Materials Science and Engineering, College of Engineering, Peking University, Beijing 100871, China

**ABSTRACT:** Transition metal dinitrides (TMDNs) have attracted increasing attention for their rich chemistry, intriguing properties, and potential applications in electronic devices and electrodes. The similarity in atomic ratio with transition-metal dichalcogenide (TMD) sheets leads to an assumption in previous studies that TMDN sheets adopt similar geometry to that of TMD sheets. Here, using global particle-swarm optimization method combined with first-principles calculations, we show a distinct structure of YN<sub>2</sub> monolayer containing isolated N<sub>2</sub> dimers labeled as O-YN<sub>2</sub>, which is dynamically, thermally and mechanically stable, and energetically favorable over the previously predicted H- and T-YN<sub>2</sub> monolayer structures. Moreover, because of its unique atomic config-



uration, the  $O-YN_2$  sheet is metallic, providing an intrinsic advantage in electrical conductivity over those semiconducting or insulating transition-metal oxides and TMD layers. In particular, we find that  $O-YN_2$  is a promising anode material for potassium ion batteries (KIBs) with competitive potassium capacity, low open-circuit voltage, and small migration barrier compared with other anode materials for potassium ion batteries, adding new features to 2D materials family.

# INTRODUCTION

Exhibiting intriguing physical and chemical features, 2D materials have attracted considerable attention in recent years. These already synthesized 2D materials like graphene,<sup>1</sup> black phosphorus,<sup>2</sup> MXene,<sup>3</sup> and transition-metal dichalcogenides (TMDs)<sup>4</sup> have shown great potentials for various applications such as field effect transistors,<sup>5</sup> p-n junctions,<sup>6</sup> and energy storage technologies such as supercapacitors<sup>7</sup> and batteries,<sup>8,9</sup> which encourage more theoretical work to predict and design new 2D materials with novel properties for expanding the 2D family. Recently, 2D transition-metal dinitrides (TMDNs) have received increasing attention since the first experimental synthesis of MoN<sub>2</sub>.<sup>10</sup> Layered bulk MoN<sub>2</sub> is known to share the same rhombohedral structure and atomic ratio with bulk MoS<sub>2</sub>, and thus it seems natural to assume that MoN<sub>2</sub> monolayer exfoliated from bulk MoN<sub>2</sub> would also inherit the structural features of MoS2-type monolayer like H- and Tconfiguration.<sup>11</sup> Therefore, H-MoN<sub>2</sub> monolayer was proposed and found to display a robust ferromagnetism with a Curie temperature over 420 K.<sup>12</sup> Moreover, it was also predicted to be a promising material for battery electrodes with high alkali metal capacities.<sup>13</sup>

These findings are very encouraging, and the extension of the research by replacing Mo with other metal elements such as Zr, Tc, and Y has been made. For instance, H-YN<sub>2</sub> monolayer was found to be half-metallic<sup>11</sup> and a good candidate for spintronic and spin caloritronic applications,<sup>14</sup> while T-YN<sub>2</sub> monolayer was suggested to be a promising Dirac half metal for high speed

spintronic devices.<sup>15</sup> However, recent studies have questioned the stability of  $\text{H-MoN}_{2^{16,17}}$  showing that the proposed structures of TMDNs by simply replacing different metal elements in MoS<sub>2</sub>-type structures are likely to be unstable. In addition, no one affirmed that they are indeed the ground states. Actually nitrogen possesses a very different chemistry compared with sulfur atom because N has fewer valence electrons and smaller covalent radius than S. Thus different geometries for 2D TMDN monolayers can be expected. Employing global structure search method<sup>18</sup> and density functional theory, we have identified the ground-state geometry of the YN<sub>2</sub> sheet with orthogonal lattice, termed as O-YN<sub>2</sub>, which is much lower in energy than H- and T-YN<sub>2</sub>. The stability of O-YN2 is confirmed by our phonon dispersion calculations, MD simulation, and mechanical parameters calculations. Different from half-metallic  $\text{H-YN}_2^{11}$  and T-YN<sub>2</sub>,<sup>15</sup> O-YN<sub>2</sub> is found to be metallic with a good electronic conductivity. Moreover, it exhibits promising potential as an anode material for potassium ion batteries with competitive K capacity, low open-circuit voltage, and small diffusion barrier.

# COMPUTATIONAL METHODS

The ground-state geometry of the  $YN_2$  monolayer is predicted by using the particle swarm optimization (CALYPSO)

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package,<sup>18</sup> which has been demonstrated to be effective in predicting energetically stable and metastable structures at given chemical composition. Atomic structure optimization, total energy, and electronic structure calculations are performed based on density functional theory (DFT), as implemented in Vienna Ab initio Simulation Package (VASP).<sup>19</sup> The projector augmented wave (PAW) method is employed to treat the interactions between ion cores and valence electrons<sup>20</sup> with a kinetic energy cutoff of 500 eV. The first Brillouin zone is sampled by a  $7 \times 5 \times 1$  k-point grid within the Monkhorst-Pack scheme.<sup>21</sup> The exchange-correlation potential is treated using Perdew-Burke-Ernzerh functional (PBE) within the generalized gradient approximation (GGA)<sup>22</sup> in most cases, while more accurate HSE06 hybrid functional<sup>23,24</sup> is used to confirm the metallic feature of the O-YN<sub>2</sub> monolayer. The atomic positions are fully relaxed until total energy converged to  $10^{-4}$  eV and atomic forces are  $<10^{-2}$  eV/Å, respectively. A large vacuum space of  $\sim 20$  Å in the perpendicular direction is used to avoid the interactions between periodic images. Phonon dispersion calculations are performed by using the PHONONPY package.<sup>25</sup> Ab initio molecular dynamics (AIMD) simulations are carried out to confirm the thermal stability. Bader charge analysis<sup>26</sup> is carried out to study the charge distribution and transfer quantitatively. The diffusion energy barrier and the minimum energy pathway of alkali metal diffusion on the O-YN2 monolayer are determined using the climbing-image nudged elastic band (CI-NEB) method.<sup>2</sup>

#### RESULTS AND DISCUSSION

**Geometry.** The most stable structure of  $YN_2$  monolayer, O-YN<sub>2</sub> is identified by using the global structure search, as shown in Figure 1. It is a quasi-2D structure with *Pmmn* space group and a thickness of 1.93 Å, where nitrogen atoms are in the form of N<sub>2</sub> dimer, very similar to the geometries of TiC<sub>2</sub> and FeC<sub>2</sub> sheets.<sup>28,29</sup> In this structure, each yttrium atom is six-foldcoordinated and each nitrogen atom is four-fold-coordinated, while the coordination number of nitrogen is three in T-YN<sub>2</sub>. One unit cell contains two yttrium and four nitrogen atoms



Figure 1. (a) Top and (b) side views of the optimized  $O-YN_2$  monolayer. (c) Charge density difference with an isovalue of 0.02 Bohr/Å<sup>3</sup>. Yellow: electron accumulation; blue: electron depletion. (d) Simulated STM images of the optimized O-YN<sub>2</sub> monolayer.

with the optimized lattice constants of a = 5.56 Å and b = 3.94 Å, which is very different from that of H-YN<sub>2</sub> and T-YN<sub>2</sub>, where there are only one yttrium and two nitrogen atoms in their unit cells with the lattice constants of 3.72 and 3.31 Å, respectively. In addition, we note that the N–N bond length of 1.32 Å in O-YN<sub>2</sub> is shorter than that of 1.43 Å in H-YN<sub>2</sub> and 2.78 Å in T-YN<sub>2</sub>, indicating that the N–N bonding in O-YN<sub>2</sub> is stronger than those in the other two isomers. The N–N bond length in O-YN<sub>2</sub> is also shorter than that in bulk PtN<sub>2</sub> (1.41 Å)<sup>30</sup> and OsN<sub>2</sub> (1.43 Å)<sup>31</sup> with N–N single bond character but longer than that of 1.23 Å in BaN<sub>2</sub> with double-bond feature,<sup>32</sup> suggesting that the N–N bond in O-YN<sub>2</sub> is between the single bond and the double bond.

On the basis of Bader charge analysis, we find that Y loses 1.85 electrons per atom, similar to the value of  $1.80 \text{ e}^-$  for Ti in TiN<sub>2</sub> with the N–N bond length 1.38 Å<sup>33</sup> but larger than that of Pt (1.05 e<sup>-</sup>) in PtN<sub>2</sub>.<sup>34</sup> To get more insight into the nature of the N–N bonding in O-YN<sub>2</sub>, the charge density difference is given in Figure 1c, which shows that electron accumulation occurs at the middle and the outer layers of the N–N bond, implying that there are  $\sigma$  bond and partially formed  $\pi$  bond within a N<sub>2</sub> dimer. The simulated scanning tunneling microscopy (STM) image (using the constant height model<sup>35</sup> with a height of 1.0 Å and a positive bias of 0.05 V) of the optimized O-YN<sub>2</sub> monolayer is given in Figure 1d for experimental comparison in the future.

To reconfirm the energetic stability of the O-YN2 sheet, we calculate the cohesive energy defined as  $E_{\rm coh} = -(E_{\rm YN_2} - nE_{\rm Y} 2nE_{\rm N}$ )/3n, where  $E_{\rm Y}$ ,  $E_{\rm N}$ , and  $E_{\rm YN_2}$  are the total energies of single Y atom, single N atom, and the O-YN<sub>2</sub> monolayer, respectively, and n is the number of YN<sub>2</sub> formula unit per unit cell. The calculated cohesive energies are 5.41, 5.24, and 4.29 eV/atom for O-YN2, H-YN2, and T-YN2, respectively, indicating that O-YN2 is the most energetically favorable structure due to the strong N-N bonding. Meanwhile, we note that the cohesive energy of O-YN<sub>2</sub> is even greater than that of some experimentally synthesized monolayers, like black phosphorus (3.48 eV/atom),<sup>2</sup> silicene (3.94 eV/atom),<sup>36</sup> and  $MoS_2$  (5.05 eV/atom).<sup>37</sup> Moreover, although the O-YN<sub>2</sub> monolayer has not been synthesized yet, it is possible to be realized experimentally from thermodynamics point of view via a direct chemical reaction:

$$Y + N_2 \rightarrow O-YN_2$$

The energy change of this reaction is defined as  $E_{\rm R} = E_{\rm YN_2} - E_{\rm Y}$ -  $E_{\rm N_2}$ , where  $E_{\rm YN_2}$  is the total energy of O-YN<sub>2</sub> per formula unit,  $E_{\rm Y}$  is the energy of a Y atom in its bulk phase, and  $E_{\rm N_2}$  is the energy of an isolated nitrogen molecule. On the basis of our DFT calculations, these values are found to be  $E_{\rm Y} = -6.43$  eV,  $E_{\rm N_2} = -16.63$  eV, and  $E_{\rm YN_2} = -24.66$  eV. Therefore, the energy change of this reaction ( $E_{\rm R}$ ) is -1.60 eV, implying that the reaction of converting yttrium and nitrogen molecule into O-YN<sub>2</sub> is exothermic, and such reaction is thermodynamically favorable in experiments. Therefore, we conclude that it is thermodynamically possible to experimentally synthesize the O-YN<sub>2</sub> monolayer

**Dynamical Stability.** To confirm the dynamical stability of the O-YN<sub>2</sub> monolayer, we first calculate its phonon dispersion. As shown in Figure 2a, the O-YN<sub>2</sub> monolayer is dynamically stable because all of the vibrational modes are real in the whole Brillouin zone. The partial density of states (PDOS) suggests



**Figure 2.** (a) Phonon spectra and phonon PDOS calculated using  $3 \times 3 \times 1$  supercell. (b) Fluctuation of total potential energy ( $4 \times 4 \times 1$  supercell) at temperature of 800 K during AIMD simulation.

that the vibrational modes below 7.5 THz consist of three acoustic bands and three optical bands, which are mainly contributed by the Y atoms due to their greater atomic number. The two highest optical vibrational modes contributed by the N<sub>2</sub> dimers are separated from the other optical modes by a large phonon gap of ~18 THz, and the frequency of ~35 THz (~1170 cm<sup>-1</sup>) is similar to that of TiN<sub>2</sub> (~1150 cm<sup>-1</sup>),<sup>33</sup> higher than that of PtN<sub>2</sub> (860 cm<sup>-1</sup>)<sup>30</sup> and lower than that of BaN<sub>2</sub> (1466 cm<sup>-1</sup>),<sup>32</sup> once again confirming that the N–N bond in the O-YN<sub>2</sub> monolayer is in between the single bond in PtN<sub>2</sub> and the double bond in BaN<sub>2</sub>.

**Thermal Stability.** We next examine the thermal stability by performing AIMD simulations. A 4 × 4 × 1 supercell containing 96 atoms is used to reduce the lattice translational constraints. The simulation is carried out with a Nosé–Hoover heat bath scheme<sup>38</sup> at 800 K for 8 ps with a time step of 1 fs. This simulation time is longer than what has been used in many previous works,<sup>29,39,40</sup> which makes the simulation more convincing. The fluctuation of the total potential energy with simulation time is plotted in Figure 2b, which shows that the average value of the total potential energy remains nearly constant during the entire simulation, confirming that the O-YN<sub>2</sub> monolayer is thermally stable at 800 K.

**Mechanical Stability and Mechanical Properties.** To further investigate how lattice distortions affect the structural stability of O-YN<sub>2</sub>, we first derive the elastic constants, which are calculated to be  $C_{11} = 152.2 \text{ N} \cdot \text{m}^{-1}$ ,  $C_{22} = 52.9 \text{ N} \cdot \text{m}^{-1}$ ,  $C_{12} = 31.9 \text{ N} \cdot \text{m}^{-1}$ , and  $C_{44} = 33.0 \text{ N} \cdot \text{m}^{-1}$ . Obviously, they satisfy the Born criteria, <sup>41,42</sup> namely,  $C_{11}$ ,  $C_{22}$ ,  $C_{44} > 0$ , and  $C_{11}C_{22} - C_{12}^2 > 0$ , suggesting that the O-YN<sub>2</sub> monolayer is mechanically stable. We then calculate the maximum value of in-plane Young's modulus of O-YN<sub>2</sub> using  $Y = (C_{11}^2 - C_{12}^2)/C_{11}$ . For comparison, the calculated results and those of some other 2D materials including H-YN<sub>2</sub>, T-YN<sub>2</sub>, TiC<sub>2</sub>, <sup>28</sup> FeC<sub>2</sub>, <sup>29</sup> MoS<sub>2</sub>, <sup>43</sup> and graphene<sup>44</sup> are summarized in Table 1. One can see that

Table 1. Mechanical Properties of the O-YN<sub>2</sub> Sheet and Some Other 2D Systems

materials	O- YN <sub>2</sub>	H- YN <sub>2</sub>	T- YN <sub>2</sub>	TiC <sub>2</sub>	FeC <sub>2</sub>	$MoS_2$	graphene
$C_{11} (N \cdot m^{-1})$	152	106	75	141	133	140	353
$C_{22}$ (N·m <sup>-1</sup> )	53	85	75	71	68	40	61
$Y(\mathbf{N}\cdot\mathbf{m}^{-1})$	146	43	66	131	98	129	342

the O-YN<sub>2</sub> sheet has a higher ideal strength than its two allotropes (H- and T-YN<sub>2</sub>), the two carbides (TiC<sub>2</sub> and FeC<sub>2</sub>) containing the C<sub>2</sub> dimers, and MoS<sub>2</sub>, reflecting the strong bonding feature of O-YN<sub>2</sub>.

**Electronic Properties.** To study the electronic properties, we calculate the electronic density of states (DOS) and the electronic band structure of the O-YN<sub>2</sub> monolayer. The results are plotted in Figure 3a,b. The O-YN<sub>2</sub> monolayer is found to be metallic as the partially occupied bands, namely, the bands numbered 3 and 4, cross the Fermi level in the Brillouin zone. The metallicity is further confirmed by using more accurate HSE06 functional.<sup>23,24</sup> Orbital-decomposed DOS suggests that the bands near the Fermi level are dominated by the N 2p (dark yellow) orbitals, while Y 4d (dark cyan) and Y 5p (blue) orbitals also make small contributions to the observed metallicity. By carefully examining the PDOS and the band structure, we clarify the interactions between the frontier orbitals of the N<sub>2</sub> dimers and Y atoms, as illustrated in Figure 3c. The ground-state electronic configuration of the isolated  $N_2$ dimer is  $(1\sigma_g)^2(1\sigma_u)^2(2\sigma_g)^2(2\sigma_u)^2(1\pi_u)^4(3\sigma_g)^2$  with the higher states  $(1\pi_{\sigma})(3\sigma_{u})$  unoccupied, and each isolated Y atom in the ground state has the electronic configuration  $[Kr]4d^{1}5s^{2}$  with its 5p orbitals unoccupied. As shown in Figure 3, the energy bands numbered 1 to 4 correspond to the four  $1\pi_{\sigma}$  states of the two N<sub>2</sub> dimers, and they hybridize with Y 4d, Y 5s, and Y 5p states, forming the two fully occupied bands (the first and second bands) and two partially occupied bands (the third and fourth bands). The fifth and sixth bands correspond to the two  $3\sigma_{\rm u}$  states of the two N<sub>2</sub> dimers with an energy slightly higher than that of the  $1\pi_{g}$  states. Bader charge analysis shows that each Y losses 1.85 electrons mainly from the outermost 5s electrons transferring to the  $1\pi_g$  states, and while the remaining ~0.15 5s electrons are shared with 4d and 5p orbitals through hybridization, especially 5p orbitals as they are closer to N<sub>2</sub> dimers. That could explain why Y 5p orbitals have a limited but observable contribution, while Y 5s (red) orbitals contribute much less to the density of states near the Fermi level.

Alkali Atom Adsorption. The metallicity of O-YN<sub>2</sub> provides an intrinsic advantage in electrical conductivity as compared with semiconducting or insulating transition-metal oxides and other TMD layers. Therefore, it may find applications in electrodes. As a matter of fact, it has been demonstrated that some TMDNs, like H-MoN<sub>2</sub>, are promising materials for battery electrodes with high alkali metal capacities<sup>13</sup> and some 2D metal carbides, such as TiC<sub>2</sub>.<sup>28</sup> are good candidates for anodes of Li-ion batteries (LIBs) with a high Li capacity and a small diffusion barrier. Considering that Y atoms have a smaller atomic number than Mo atoms and O-YN<sub>2</sub> shares a similar structure with TiC<sub>2</sub>, we expect that the O-YN<sub>2</sub> monolayer can be also used in electrodes for alkali metal ion batteries.

To determine the most favorable adsorption site of a single alkali atom (Li, Na, and K, respectively), four possible adsorption sites are considered as depicted in Figure 4, where

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Figure 3. (a) PDOS and (b) electronic band structure of the O-YN<sub>2</sub> monolayer. (c) Schematic diagram showing the interactions between the frontier orbitals of the  $N_2$  dimers and Y atoms.



Figure 4. Considered adsorption sites on the O-YN<sub>2</sub> monolayer.

 $S_1$  is the hollow site of the four neighboring N<sub>2</sub> dimers,  $S_2$  is the bridge site of the  $N_2$  dimer,  $S_3$  is the on-top site of the Y atom that is between the two parallel N2 dimers lying in two neighboring lines, and  $S_4$  is the on-top site of the Y atom that is between the two neighboring N<sub>2</sub> dimers lying alone a line. To obtain reliable results, full structural optimizations are carried out for all of the adsorption configurations with a  $2 \times 2 \times 1$ supercell of the O-YN2 monolayer. The most favorable adsorption configuration is identified by comparing the adsorption energy, defined as  $E_{\rm Ad}$  =  $E_{\rm M+YN_2}$  –  $E_{\rm YN_2}$  –  $E_{\rm AA}$ where  $E_{\rm YN_2}$  and  $E_{\rm YN_2+M}$  are the total energies of the O-YN<sub>2</sub> monolayer supercell before and after the adsorption, respectively, and  $E_A$  represents the energy per alkali atom in its corresponding bulk phase. The calculated results are listed in Table 2. One can see that  $S_3$  is the most favorable adsorption site for the three kinds of alkali atoms, and all of the adsorption configurations for K are energetically more favorable than those

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Table 2. Adsorption Energy (in eV) of a Single Alkali Atom
(Li, Na, and K) on the O-YN <sub>2</sub> Monolayer for Different
Adsorption Sites $(S_1, S_2, S_3, \text{ and } S_4)$ , and the Corresponding
Distance (in Å) between the Atom and the O-YN <sub>2</sub>
Monolayer

	0	0	6	0
	$S_1$	$S_2$	S <sub>3</sub>	S <sub>4</sub>
Li	0.37(eV)	-0.54 (eV)	-0.62 (eV)	-0.17(eV)
	2.29 (Å)	2.79 (Å)	2.20 (Å)	2.22(Å)
Na	0.12 (eV)	-0.13 (eV)	-0.46 (eV)	0.11 (eV)
	2.86 (Å)	3.14 (Å)	2.61 (Å)	2.82 (Å)
Κ	-0.37 (eV)	-0.63 (eV)	-0.90 (eV)	-0.52 (eV)
	3.15 (Å)	3.51 (Å)	3.09 (Å)	3.15 (Å)

for Li and Na, respectively, indicating a better ability of K to bind to the  $O-YN_2$  monolayer as compared with Li and Na.

Potential Application as an Anode Material for KIBs. The good ability to absorb K atoms suggests that the O-YN<sub>2</sub> monolayer is a potential candidate for electrodes for potassium ion batteries (KIBs). As an alternative to the widely used LIBs, KIBs would serve more as large-scale batteries for stationary storage. While one of the biggest challenges for practical uses of KIBs is to find ideal anode materials. For example, the widely used graphite anodes for LIBs are not suitable for KIBs<sup>45,46</sup> due to the huge volume expansion. In the following, we systematically explore the possibility of the O-YN<sub>2</sub> monolayer as an anode material for KIBs by examining the diffusion and adsorption behavior of K atoms on this monolayer and study the relative electrochemical properties of the K adsorbed O-YN<sub>2</sub>.

The rate performance of an anode material is mainly determined by the mobility of the intercalating ions. Therefore, we estimate the diffusion behavior of K atoms on the O-YN<sub>2</sub> monolayer by employing the CI-NEB method. We consider three diffusion paths that connect the two neighboring most preferable K adsorption sites  $(S_3)$ , as indicated in Figure 5a. According to Figure 5b, Path 1 is found to have the lowest



Figure 5. (a) Considered diffusion paths of K on the surface of the O-YN<sub>2</sub> monolayer. (b) Corresponding diffusion energy barrier profiles.



Figure 6. (a) Geometry of the K-adsorbed O-YN<sub>2</sub> monolayer (YN<sub>2</sub>K). (b) Electron localization function of the (010) section of YN<sub>2</sub>K. (c) DOS of YN<sub>2</sub>K.

diffusion barrier of 0.27 eV and the shortest diffusion length of 4.21 Å. The energy barrier is much smaller than that of H-MoN<sub>2</sub> (0.49 eV),<sup>13</sup> indicating a very good conductivity of the K ions on the O-YN<sub>2</sub> monolayer, and excellent charge–discharge rate can be expected for the O-YN<sub>2</sub> monolayer when it is used as an anode for KIBs.

Next we study the adsorption of K with high concentration. For the O-YN<sub>2</sub> monolayer, we increase the concentration of K from the stoichiometry of  $Y_8N_{16}K$  to  $YN_2K$ . As shown in Figure 6a, the most favorable adsorption site of K is again determined to be  $S_3$  by following the same procedure, and the average  $E_{Ad}$  is calculated to be -0.48 eV, demonstrating the thermodynamic stability of this adsorption configuration. On the basis of Bader charge analysis, we find that each K atom transfers 0.63 electrons to the O-YN<sub>2</sub> monolayer, suggesting that K atoms are in the cationic state and chemically adsorbed onto the O-YN<sub>2</sub> monolayer. In Figure 6b we display the electron localization function (ELF) of the (010) section of YN<sub>2</sub>K. According to this

graph we find no electron accumulation between K atoms, excluding the possibility that K atoms form clusters and ensuring that they all bind to the O-YN<sub>2</sub> substrate. To study the effect of high K concentration on the electronic structure, we calculated the electronic density of states of YN2K. According to Figure 6c, the calculated DOS clearly exhibits metallic character, which ensures good electronic conduction when used in battery electrodes. Considering the aforementioned adsorption configuration of YN2K, the theoretical K capacity is calculated to be 229 mAh/g, which is slightly larger than that of  $Ti_{3}C_{2}$  (192 mAh/g)<sup>47</sup> and Sn-C alloy (190 mAh/g).<sup>48</sup> Although O-YN<sub>2</sub> is seemingly inferior to H-MoN<sub>2</sub> (432 mAh/ g)<sup>13</sup> in capacity, the open-circuit voltage (OCV) is 0.48 V, which is much more suitable to serve as an anode material as compared with H-MoN<sub>2</sub> with an OCV of 1.11 V,<sup>13</sup> and according to the discussion above, the diffusion barrier of O-YN<sub>2</sub> is also much smaller than that of H-MoN<sub>2</sub>, resulting in better rate performance. Considering the fact that the stability

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of O-YN<sub>2</sub> has been confirmed by our discussion above while the stability of H-MoN<sub>2</sub> is still being questioned, <sup>16,17</sup> we believe that the O-YN<sub>2</sub> monolayer is more promising to serve as a future 2D anode material for KIBs than H-MoN<sub>2</sub>.

## CONCLUSIONS

In summary, stimulated by the intriguing properties and promising applications of previously proposed TMDNs and the recent doubt about the stability of H-MoN<sub>2</sub>, we carried out a global structure search and identified the ground-state structure of YN<sub>2</sub> monolayer, named O-YN<sub>2</sub>, which is energetically more stable than previously proposed H- and T-YN<sub>2</sub> structures, displaying a metallic feature instead of half-metallicity, as found in H-YN2 and T-YN2, and showing dynamical, thermal, and mechanical stabilities. We further demonstrated that the O-YN<sub>2</sub> monolayer exhibits excellent adsorption ability toward potassium and thus can serve as a promising anode material for potassium ion batteries with competitive theoretical potassium capacity, low open-circuit voltage, and small diffusion barrier. Our study not only expands the family of 2D materials but also indicates that TMDNs can show different geometries with unique features as compared with the widely studied TMDs.

## AUTHOR INFORMATION

## **Corresponding Author**

\*E-mail: qianwang2@pku.edu.cn.

## ORCID <sup>©</sup>

Qian Wang: 0000-0002-9766-4617

#### Notes

The authors declare no competing financial interest.

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