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# First principles study of optoelectronic and photocatalytic performance of novel transition metal dipnictide $XP_2$ ( $X = \text{Ti, Zr, Hf}$ ) monolayers

Sheraz Ahmad,<sup>†a</sup> Ismail Shahid,<sup>†a</sup> Nasir Shehzad,<sup>b</sup> W. Khan,<sup>©\*c</sup> H. U. Din,<sup>\*c</sup> M. Idrees,<sup>d</sup> B. Amin<sup>©d</sup> and A. Laref<sup>©e</sup>

Low cost and highly efficient two dimensional materials as photocatalysts are gaining much attention to utilize solar energy for water splitting and produce hydrogen fuel as an alternative to deal with the energy crisis and reduce environmental hazards. First principles calculations are performed to investigate the electronic, optical and photocatalytic properties of novel two dimensional transition metal dipnictide  $XP_2$  ( $X = \text{Ti, Zr, Hf}$ ) monolayers. The studied single layer  $XP_2$  is found to be dynamically and thermally stable.  $\text{TiP}_2$ ,  $\text{ZrP}_2$  and  $\text{HfP}_2$  systems exhibit semiconducting nature with moderate indirect band gap values of 1.72 eV, 1.43 eV and 2.02 eV, respectively. The solar light absorption is found to be in energy range of 1.65–3.3 eV. All three  $XP_2$  systems (at pH = 7) and the  $\text{HfP}_2$  monolayer (at pH = 0) that straddle the redox potentials, are promising candidates for the water splitting reaction. These findings enrich the two dimensional family and provide a platform to design novel devices for emerging optoelectronic and photovoltaic applications.

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## Introduction

The reduction in fossil fuels and challenges to energy sources have forced the scientific society to search for environment friendly and efficient green energy fuels for sustainable development of a clean society.<sup>1</sup> Hydrogen is considered as an ideal energy carrier source due to its abundance on earth, low pollution emission<sup>2</sup> and highest energy per mass ratio. To produce hydrogen from water, photocatalytic water splitting is the most favorable method. For a few decades, researchers have been devoted to producing some novel metal-based inexpensive environment friendly photocatalytic materials.<sup>3</sup> Two-dimensional materials like hexagonal boron nitride (h-BN) and transition metal dichalcogenides (TMDCs) have invoked considerable interest after the successful development of graphene in 2004.<sup>4</sup> Single layer transition metal dichalcogenides have tremendous applications like optoelectronics, spintronics, valleytronics, photovoltaic devices, gas sensing, and catalysis

due to their suitable band gap, good mechanical properties and absorption coefficients.<sup>5–8</sup> The developed nano- and meso-structures, phosphides and phosphates have shown good flexibility and electrical conductivity<sup>9</sup> in comparison with oxides and polymers, and are ideal for storing electrochemical energy based on faradaic redox reactions.<sup>10</sup>

Ranking 10<sup>th</sup> in the abundance in the earth crust, phosphorus is considered very effective for hydrogen evolution<sup>11</sup> and reports have shown that P played main role in photo catalysts.<sup>12</sup> Due to low band gap, good stability and electrical conductivity, transition metal phosphides (TMPs) are considered as good semiconductor materials.<sup>13</sup> Many compounds of phosphorus including phosphides and metal phosphates have been studied for super capacitors,<sup>14</sup> lithium ion batteries<sup>15</sup> and catalysts.<sup>16</sup> Phosphorus make variety of phosphides when react with various elements in periodic table.<sup>17</sup> For making transition metal phosphides, large atomic radius (0.109) of phosphorus makes it favorable in designing various crystal structures.<sup>9</sup> Doping of some noble metals Pt, Pd, Au make photocatalytic material very efficient for photocatalytic hydrogen production<sup>18,19</sup> but their applications are limited due to high cost.<sup>20</sup> Therefore, search for more effective and cheap catalysts are very essential and highly demanding.<sup>21</sup>

Generally, two conditions must be fulfilled for photocatalytic material: (1) its conduction band edge should be more negative than  $\text{H}_2$  energy level, (2) the valence band edge must be lower than the energy level of oxygen.<sup>22</sup> Despite of efficient performance of hydrogen evolution reaction (HER) for using catalyst in water splitting, controlling the basic structural composition

<sup>a</sup>School of Materials Science and Engineering, Computational Centre for Molecular Science, Institute of New Energy Material Chemistry, Nankai University, Tianjin 300350, P. R. China

<sup>b</sup>School of Physics, Nankai University, Tianjin 300071, P. R. China

<sup>c</sup>Department of Physics, Bacha Khan University, Charsadda, KP, Pakistan. E-mail: haleem.uddin@yahoo.com

<sup>d</sup>Department of Physics, Abbottabad University of Science & Technology, Havelian, Abbottabad, KP, Pakistan

<sup>e</sup>Department of Physics and Astronomy, College of Science, King Saud University, Riyadh, 11451, Saudi Arabia

<sup>†</sup> These authors contributed equally to this work.



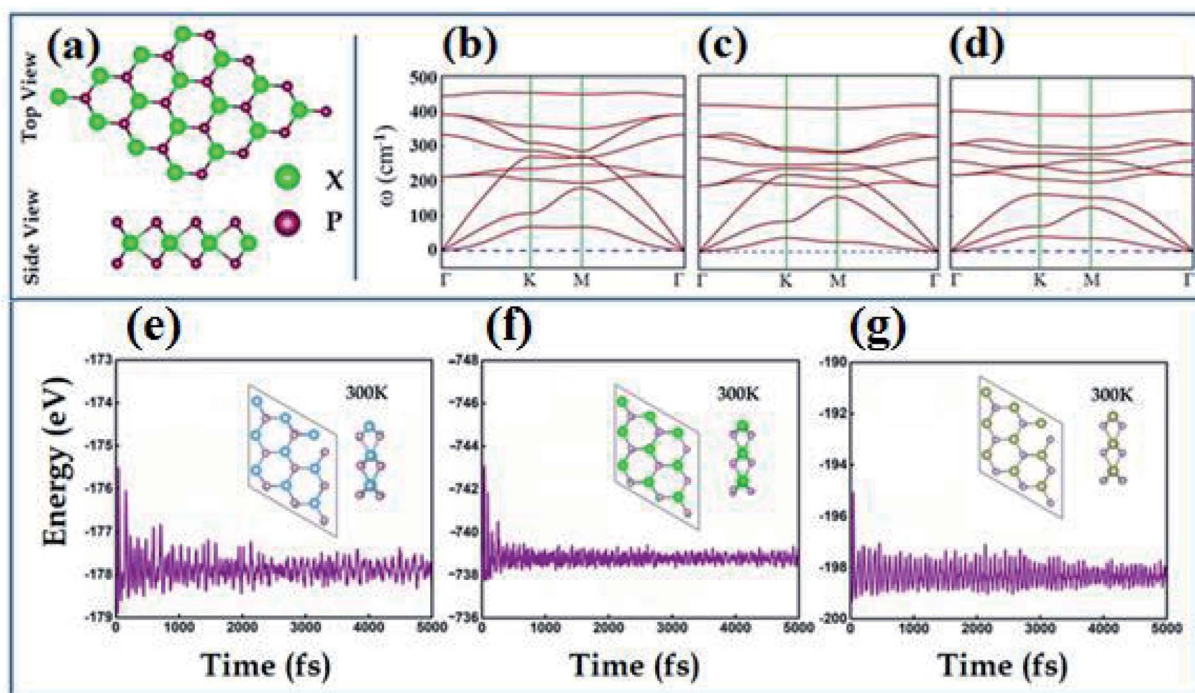


Fig. 1 (a) Top and side view of  $XP_2$  monolayers, (b–d) phonon band structure and (e–g) AIMD calculated energy *versus* time plots with insets show the side and top view at 300 K of  $TiP_2$ ,  $ZrP_2$  and  $HfP_2$ , respectively.

is still a challenge.<sup>23,24</sup> C. Y. Son and coworkers have synthetically developed FeP and  $FeP_2$  nanowires and demonstrated high electro-catalytic performance for P-rich  $FeP_2$  nanowires in acidic and basic solution.  $FeP_2$  revealed remarkable performance for water splitting. Transition metal phosphides have been discovered recently to decompose methyl orange efficiently and to produce hydrogen by photocatalytic activity.<sup>25</sup> These findings have opened new windows for searching of novel photocatalysts and screening of new materials.<sup>26,27</sup> Recent reports show  $MoP_2$  is used to produce hydrogen as semi-metallic photocatalyst.  $MoP_2$  nanosheets possess excellent electronic properties with high active site density exposure.<sup>28</sup> Many early transition metal dipnictides (TMDPs) have been explored in orthorhombic and  $OsGe_2$  or  $MoP_2$  type-phase.<sup>28–36</sup> However, TMDPs with hexagonal graphene-like structure remains unexplored.

In this paper, we theoretically studied structural, electronic, optical, and photocatalytic properties of novel 2D transition metal dipnictides  $XP_2$  ( $X = Ti, Zr, Hf$ ). Our results show that  $XP_2$  ( $X = Ti, Zr, Hf$ ) with stable graphene-like hexagonal geometry are semiconductors with moderate band gaps which show good optical activity in visible and near ultraviolet region. Furthermore, the band edge positions straddle the water redox potential, predicting  $XP_2$  monolayers as suitable candidates for photocatalytic water splitting.

## Computational details

The projector augmented plane wave (PAW)<sup>37,38</sup> scheme was employed using density functional theory (DFT) implemented in Vienna *ab initio* simulation package (VASP).<sup>39,40</sup> The electronic band structure is calculated using Perdew–Burke–

Ernzerhof (PBE)<sup>41</sup> functional. The semi-empirical van der Waals (vdW) corrections are considered as proposed by Grimme.<sup>42,43</sup> We relaxed  $XP_2$  monolayers and converged energy to  $10^{-5}$  eV and residual forces to  $10^{-4}$  eV  $\text{\AA}^{-1}$ . A  $\Gamma$ -centered Monkhorst–Pack  $k$ -meshes of  $6 \times 6 \times 1$  were used for structural relaxation of monolayers and for optimized structures upgraded to  $12 \times 12 \times 1$  with 500 eV was used as plane-wave cutoff energy. A vacuum layer of 25  $\text{\AA}$  in direction of out-of-plane was used to preclude interaction between layers. The converged PBE wave functions were used as starting point of Heyd–Scuseria–Ernzerhof (HSE06).<sup>44</sup> VASP associated phonopy code was used for phonon spectra calculation. Harmonic interatomic force constant is used as input *via* Phonopy code that is attained by density functional perturbation theory (DFPT).<sup>45,46</sup> A  $5 \times 5 \times 1$  supercell with energy cut-off (500 eV) was used for phonon spectrum.

## Results and discussion

The transition metal dipnictides  $XP_2$  ( $X = Ti, Zr$ , and  $Hf$ ) like transition metal dichalcogenides<sup>47,48</sup> exhibit the same hexagonal structure having trigonal prismatic 2H phase with

**Table 1** The calculated lattice constant ( $a$  in  $\text{\AA}$ ), bond length (P–X in  $\text{\AA}$ ), bond angle ( $\theta_{P-X-P}$  in degree) between X and P atoms, and band gap ( $E_g$  in eV) using PBE- and HSE06 functionals, of  $XP_2$  monolayers

Monolayer	$a$ ( $\text{\AA}$ )	P–X ( $\text{\AA}$ )	$(\theta_{P-X-P})$	$E_{g-PBE}$ (eV)	$E_{g-HSE06}$ (eV)
$TiP_2$	3.80	2.47	$54.73^\circ$	0.70	1.72
$ZrP_2$	4.10	2.63	$51.99^\circ$	0.67	1.43
$HfP_2$	4.00	2.59	$53.93^\circ$	1.23	2.02



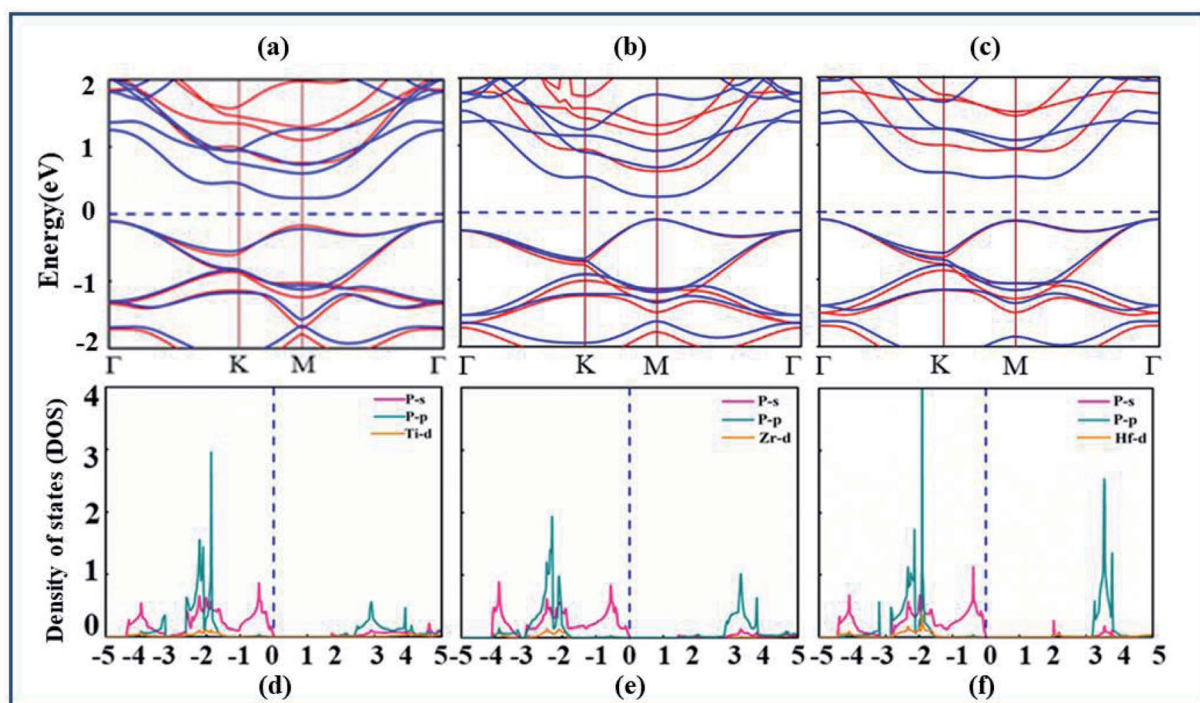


Fig. 2 (a–c) The calculated electronic band structure represented by blue solid lines (PBE-functional) and red solid lines (HSE06 functional), and (d–f) partial density of states (PDOS) of  $\text{TiP}_2$ ,  $\text{ZrP}_2$  and  $\text{HfP}_2$ , respectively.

transition metal (X-atom) sandwiched between two phosphorus atoms as shown in Fig. 1(a). The optimized lattice parameters, bond lengths ( $d_{\text{X-P}}$ ), bond angle ( $\theta_{\text{P-X-P}}$ ) and calculated band gap using PBE and HSE06 schemes are listed in Table 1. The phonon band spectrum of  $\text{XP}_2$  ( $\text{X} = \text{Ti}, \text{Zr}, \text{Hf}$ ), displayed in Fig. 1(b–d), consists of three lowest frequency acoustic modes with no imaginary frequency at the  $\Gamma$ -point. This confirms that all studied monolayers are dynamically stable. Further, the thermal stability of all  $\text{XP}_2$  monolayers has been ascertained by

performing *ab initio* molecular dynamics (AIMD) calculations at room temperature. The snapshots of the final geometry of  $\text{XP}_2$  monolayers with energy fluctuation *versus* time (5000 ps) have been shown in Fig. 1(e–g). All single layer  $\text{XP}_2$  have no considerable energy fluctuations and possess no broken bonds in the final structures at 300 K, indicating the experimental fabrication of understudy systems.

After confirmation of structural stability and manufacturing possibility of monolayers  $\text{XP}_2$ , electronic band structure and density of states (DOS) are calculated (as displayed in Fig. 2(a–

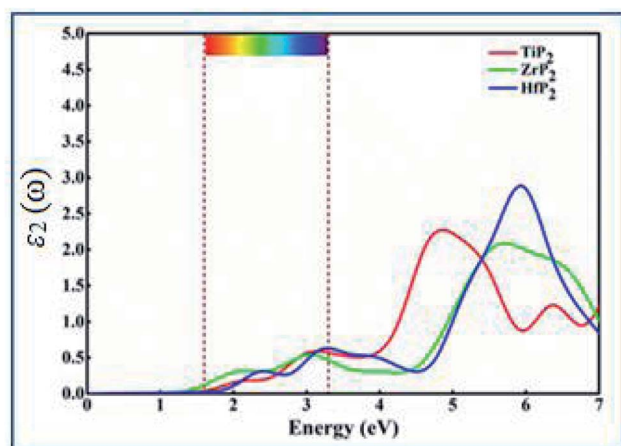


Fig. 3 Imaginary part of the dielectric constant ( $\epsilon_2(\omega)$ ) as a function of photon energy for the  $\text{XP}_2$  ( $\text{X} = \text{Ti}, \text{Zr}$ , and  $\text{Hf}$ ) monolayer obtained from the average of  $x$ ,  $y$ , and  $z$  polarization vectors. The area between the two brown dashed lines is the energy range of visible light.

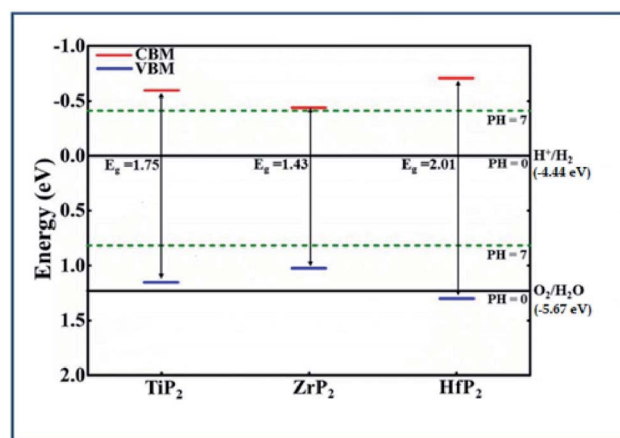


Fig. 4 Band edge locations of the three of  $\text{XP}_2$  ( $\text{X} = \text{Ti}, \text{Zr}$ , and  $\text{Hf}$ ) monolayers relative to the water oxidation ( $\text{O}_2/\text{H}_2\text{O}$ ) and reduction ( $\text{H}^+/\text{H}_2$ ) potentials at  $\text{pH} = 0$  and 7 levels.





c)) to gain deep insight into their electronic properties. According to our calculations,  $\text{XP}_2$  ( $\text{X} = \text{Ti}, \text{Zr}, \text{Hf}$ ) monolayers reveal semiconducting behavior with indirect band gap of 0.70 eV, 0.67 eV and 1.23 eV respectively with PBE functional. In addition, the hybrid functional (HSE06)<sup>44</sup> is used to make correction to the self-interaction (SIF) error which underestimates band gap. The calculated band structure of  $\text{XP}_2$  monolayers exhibits the same band character with larger band gap values 1.72 eV ( $\text{TiP}_2$ ), 1.43 eV ( $\text{ZrP}_2$ ) and 2.02 eV ( $\text{HfP}_2$ ). Red and blue colors represent HSE06 and PBE band structure as shown in Fig. 2(a–c). For  $\text{TiP}_2$  and  $\text{ZrP}_2$  systems, the conduction band minimum (CBM) lies at the M-point and valence band maximum (VBM) lies at the  $\Gamma$ -point of the Brillouin zone, representing an indirect band nature. In case of  $\text{HfP}_2$ , CBM lies between M and  $\Gamma$  point while VBM lies at  $\Gamma$ -point of the Brillouin zone indicating an indirect semiconducting behavior. Similar trend is observed for other two dimensional materials.<sup>25,28,49,50,52,54</sup>

The analysis of individual states contributing near the Fermi level ( $E_F$ ) is obtained by plotting the partial density of states (PDOS) of under study systems. The X-d (orange), P-s (pink), P-p (cyan) orbitals and Fermi level ( $E_F$ ) represented by blue dashed line are shown in Fig. 2(d–f). The PDOS of X-s and X-p states found deeper in energy region are avoided here. It is obvious from Fig. 2(d–f) that both VBM and CBM are predominantly attributed by P-s orbital of all  $\text{XP}_2$  systems.

The optical behavior of  $\text{XP}_2$  systems is crucial for exploring the absorption and conversion of sunlight into electric current for various applications. Complex dielectric function specifically describes optical properties by formula  $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$ .<sup>49</sup> In the present work, the optical absorption spectra in terms of imaginary part  $\epsilon_2(\omega)$  is calculated between 0–7.0 eV energy range, as shown in Fig. 3. From  $\epsilon_2(\omega)$  spectra of all  $\text{XP}_2$  systems, a considerable visible light absorption is found between 1.65–3.3 eV energy range, suggesting these monolayers as promising candidates for solar energy absorber and photovoltaic applications.

Generally, the band gap of a material must be larger than 1.23 eV to perform the photocatalytic activity for water splitting. Using HSE06 functional, the calculated band gap values of  $\text{XP}_2$  monolayers exceed free energy value (1.23 eV), implying that  $\text{XP}_2$  monolayers satisfies the water splitting reaction. The valence band edge ( $E_{\text{VB}}$ ) and conduction band edge ( $E_{\text{CB}}$ ) positions are obtained by using HSE06 functional, schematically represented in Fig. 4. The standard redox potentials for photocatalytic water splitting mechanism are calculated by:

$E_{\text{O}_2/\text{H}_2\text{O}} = -5.67 \text{ eV} + \text{pH} \times 0.059 \text{ eV}$  and  $E_{\text{H}^+/\text{H}_2} = -4.44 \text{ eV} + \text{pH} \times 0.059 \text{ eV}$ .<sup>49–53</sup> Therefore, we considered redox potential levels for water as shown in Fig. 4. For  $\text{HfP}_2$  monolayer, the band edge potentials (both  $E_{\text{VB}}$  and  $E_{\text{CB}}$ ) straddle the standard redox potentials at  $\text{pH} = 0$ . However, the valence band edge of  $\text{TiP}_2$  and  $\text{ZrP}_2$  monolayers found above the standard oxidation potential thus, fails to perform oxidation evolution reaction at  $\text{pH} = 0$ . More interestingly, all  $\text{XP}_2$  monolayers with both  $E_{\text{VB}}$  and  $E_{\text{CB}}$  located below and above the standard redox potentials at  $\text{pH} = 7$ , indicates the ability to dissociate water into  $\text{H}^+/\text{H}_2$  and  $\text{O}_2/\text{H}_2\text{O}$  under the irradiation of sun light. Similar behavior

has also been reported in other literature.<sup>27,49–54</sup> These findings predict  $\text{XP}_2$  monolayers as efficient candidates for photocatalysis and photovoltaic applications.

## Conclusion

In summary, the first principles calculations are performed to investigate the structural, electronic, optical properties and photocatalytic activity of transition metal dipnictides  $\text{XP}_2$  ( $\text{X} = \text{Ti}, \text{Zr}, \text{Hf}$ ) monolayers. All single layer systems are dynamically and thermally stable. Two-dimensional  $\text{TiP}_2$ ,  $\text{ZrP}_2$  and  $\text{HfP}_2$  are indirect semiconductors (with band gap values 1.72 eV, 1.43 eV and 2.02 eV, respectively) with both VBM and CBM mainly attributed by P-s state. A considerable absorption of solar light is found between 1.65–3.3 eV. More interestingly, all  $\text{XP}_2$  systems (at  $\text{pH} = 7$ ) and  $\text{HfP}_2$  monolayer (at  $\text{pH} = 0$ ) are capable to perform redox reactions of water splitting. These results pave the path for designing future optoelectronic and photovoltaic devices.

## Conflicts of interest

There is no conflict of interest.

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