Intrinsic piezoelectricity in monolayer MSi$_2$N$_4$ (M = Mo, W, Cr, Ti, Zr and Hf)

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Abstract – Motivated by experimentally synthesized MoSi$_2$N$_4$ (HONG Y. L. et al., Science, 369 (2020) 670), the intrinsic piezoelectricity in monolayer MSi$_2$N$_4$ (M = Mo, W, Cr, Ti, Zr and Hf) are studied by density functional theory (DFT). Among the six monolayers, CrSi$_2$N$_4$ has the best piezoelectric strain coefficient $d_{11}$ of 1.24 pm/V, and the second is 1.15 pm/V for MoSi$_2$N$_4$. Taking MoSi$_2$N$_4$ as an example, strain engineering is applied to improve $d_{11}$. It is found that tensile biaxial strain can enhance $d_{11}$ of MoSi$_2$N$_4$, and the $d_{11}$ at 4% strain can improve by 107% with respect to the unstrained one. By replacing the N by P or As in MoSi$_2$N$_4$, the $d_{11}$ can be raised substantially. For MoSi$_2$P$_4$ and MoSi$_2$As$_4$, the $d_{11}$ is as high as 4.93 pm/V and 6.23 pm/V, which is mainly due to smaller $C_{11} - C_{12}$ and very small minus or positive ionic contribution to piezoelectric stress coefficient $e_{11}$ with respect to MoSi$_2$N$_4$. The discovery of this piezoelectricity in monolayer MSi$_2$N$_4$ enables active sensing, actuating and new electronic components for nanoscale devices, and is recommended for experimental exploration.

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Introduction. – Piezoelectric materials can convert mechanical energy into electrical energy and vice versa, and the piezoelectricity of two-dimensional (2D) materials has been widely investigated [1] in recent years. Experimentally, the existence of piezoelectricity of MoS$_2$ [2,3], MoSe$_2$ [4] and In$_2$Se$_3$ [5] has significantly promoted the development of the piezoelectricity of 2D materials. It has been reported that a large number of 2D materials have significant piezoelectric coefficients, such as transition metal dichalcogenides (TMD), Janus TMD, group IIA and IIIB metal oxides, group-V binary semiconductors and group III-V semiconductors [6–15], the monolayers SnSe, SnS, GeSe and GeS of which possess giant piezoelectricity, as high as 75–251 pm/V [12]. The intrinsic piezoelectricity has also been predicted in allotropes of phosphorus with remarkable stability [16]. Due to different crystal symmetry, an only in-plane piezoelectricity, both in-plane and out-of-plane piezoelectricity, or a pure out-of-plane piezoelectricity can exist, and the corresponding example is TMD monolayers [11], many 2D Janus materials [6,9] and penta-graphene [10]. The strain-tuned piezoelectric response of MoS$_2$ [17], AsP [7], SnSe [7] and Janus TMD monolayers [18] have been performed by the first-principle calculations, and it is proved that strain can improve the piezoelectric strain coefficients.

Recently, the layered 2D MoSi$_2$N$_4$ and WS$_2$N$_4$ have been synthesized by chemical vapor deposition (CVD) [19], which opens up a new, large family of 2D materials. Many other 2D materials with a general formula of MA$_2$Z$_4$ have been predicted by DFT calculations [19], where M represents an early transition metal (W, V, Nb, Ta, Ti, Zr, Hf, or Cr). A is Si or Ge, and Z stands for N, P, or As. And then twelve kinds of 2D family MA$_2$Z$_4$ are proposed with $\alpha_i$ and $\beta_i$ (i = 1 to 6) phases by intercalating the MoS$_2$-type MZ$_2$ monolayer into the InSe-type A$_2$Z$_2$ monolayer [20]. In this work, the piezoelectric properties

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of monolayer MSi$_2$N$_4$ ($M = \text{Ti, Zr, Hf, Cr, Mo and W}$) are studied by using density functional perturbation theory (DFPT) [21]. The independent in-plane piezoelectric constants $d_{11}$ are predicted to be 0.777 pm/V to 1.241 pm/V, which are smaller than the ones of many other 2D materials [6,9,11–13]. Using MoSi$_2$N$_4$ as an example, strain engineering is proposed to produce improved piezoelectric properties. It is found that increasing strain can improve $d_{11}$ due to reduced $C_{11} - C_{12}$ and enhanced $e_{11}$, and the band gap decreases. Calculated results show that MoSi$_2$P$_4$ and MoSi$_2$As$_4$ have much better $d_{11}$ than MSi$_2$N$_4$ ($M = \text{Ti, Zr, Hf, Cr, Mo and W}$), which is mainly because they are much softer, and their ionic parts give much smaller negative contribution (MoSi$_2$P$_4$) or positive contribution (MoSi$_2$As$_4$) to $e_{11}$. Our calculations show that the MA$_2$Z$_4$ ($M = \text{Ti, Zr, Hf, Cr, Mo or W}; Z = \text{Si or Ge};$ and $Z = \text{N, P or As}$) materials may be promising candidates for piezoelectric applications.

**Computational detail.** – We perform DFT calculations [22] using the projector-augmented wave method as implemented in the plane-wave code VASP [23–25]. For the structural relaxation and the calculations of the elastic and piezoelectric tensors, we use the popular generalized gradient approximation of Perdew, Burke and Ernzerhof (GGA-PBE) [26] as the exchange-correlation functional. For energy band calculations, the spin orbital coupling (SOC) is also taken into account. A cutoff energy of 500 eV for the plane wave basis set is used to ensure accurate DFT calculations. A vacuum spacing of more than 32Å is adopted to reduce the interactions between the layers, which is key to attain accurate $e_{ij}$. The total energy convergence criterion is set to $10^{-8}$ eV, and the Hellmann-Feynman forces on each atom are less than 0.0001 eV Å$^{-1}$. The coefficients of the elastic stiffness tensor $C_{ij}$ are calculated by using strain-stress relationship (SSR), and the piezoelectric stress coefficients $e_{ij}$ are attained by the DFPT method [21]. The Brillouin zone sampling is done using a Monkhorst-Pack mesh of $15 \times 15 \times 1$ for $C_{ij}$, and $9 \times 16 \times 1$ for $e_{ij}$. The 2D elastic coefficients $C_{ij}^{\text{D}}$ and piezoelectric stress coefficients $e_{ij}^{\text{D}}$ have been renormalized by the length of unit cell along the z-direction ($L_z$): $C_{ij}^{\text{D}} = L_zC_{ij}^\text{elc}$ and $e_{ij}^{\text{D}} = L_ze_{ij}^\text{elc}$.

**Symmetry analysis.** – The relaxed-ion piezoelectric stress tensors $e_{ijk}$ and strain tensor $d_{ijk}$, from the sum of ionic and electronic contributions, are defined as

$$e_{ijk} = \frac{\partial P_i}{\partial \varepsilon_{jk}} = e_{ijk}^\text{elc} + e_{ijk}^\text{ion},$$

and

$$d_{ijk} = \frac{\partial P_i}{\partial \sigma_{jk}} = d_{ijk}^\text{elc} + d_{ijk}^\text{ion},$$

where $P_i$, $\varepsilon_{jk}$ and $\sigma_{jk}$ are polarization vector, strain and stress, respectively. The $d_{ijk}$ and $e_{ijk}$ are related via the elastic stiffness tensor $C_{ijkl}$. Monolayer MSi$_2$N$_4$ belongs to the 6$m_2$ point group. Employing the Voigt notation, if we only consider in-plane strain components [6,11–14] for 2D materials, $e_{ij}, d_{ij}$ and $C_{ij}$ become

$$
\begin{pmatrix}
e_{11} & -e_{11} & 0 \\
0 & 0 & -e_{11} \\
0 & 0 & 0
\end{pmatrix},
\begin{pmatrix}
d_{11} & -d_{11} & 0 \\
0 & 0 & -2d_{11} \\
0 & 0 & 0
\end{pmatrix},
\begin{pmatrix}
C_{11} & C_{12} & 0 \\
C_{12} & C_{11} & 0 \\
0 & 0 & \frac{C_{11} - C_{12}}{2}
\end{pmatrix}.
$$

Here, the only in-plane $d_{11}$ is derived by $e_{ik} = d_{ij}C_{jk}$:

$$d_{11} = \frac{e_{11}}{C_{11} - C_{12}}. \tag{6}$$

**Main calculated results and analysis.** – The geometric structure of the MSi$_2$N$_4$ monolayer is plotted in fig. 1, which consists of seven atomic layers of N-Si-N-M-N-Si-N (a MN$_2$ layer sandwiched between two Si-N bilayers). The optimized structural parameters of MSi$_2$N$_4$ ($M = \text{Ti, Zr, Hf, Cr, Mo and W}$) (in table $1$) agree well with the previous calculated results [19]. The electronic band structures of these monolayers are also calculated using GGA and GGA+SOC, and the representative HSi$_2$N$_4$ and WSi$_2$N$_4$ monolayers are shown in fig. 2. The energy bands of MSi$_2$N$_4$ ($M = \text{Ti, Zr, Hf, Cr, Mo and W}$) near the Fermi level have M-d character. Compared to MSi$_2$N$_4$ ($M = \text{Ti, Zr, Hf}$), two additional electrons are added for MSi$_2$N$_4$ ($X = \text{Ti, Zr, Hf}$). For MSi$_2$N$_4$ ($M = \text{Cr, Mo and W}$) near the Fermi level have M-d character. Compared to MSi$_2$N$_4$ ($M = \text{Ti, Zr, Hf}$), two additional electrons are added for MSi$_2$N$_4$ ($X = \text{Ti, Zr, Hf}$).

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1. See the SM for energy band structures of monolayer MSi$_2$N$_4$ ($X = \text{Ti, Zr, Hf, Cr, Mo, W}$) and monolayer MoSi$_2$N$_4$ with strain from $-4\%$ to $4\%$.  

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Table 1: For monolayer MSi$_2$N$_4$ (M = Ti, Zr, Hf, Cr, Mo and W), the lattice constants $a_0$ (Å), the height $h$ (Å), the GGA gap $\Delta$ (eV), the GGA+SOC gap $\Delta_{soc}$ (eV), the spin-orbital splitting at K point $\Delta$ (eV), the elastic constants $C_{11} - C_{12}$ (Nm$^{-1}$), the piezoelectric coefficients $e_{11}$ (10$^{-10}$ C/m) and $d_{11}$ (pm/V).

- **TiSi$_2$N$_4**: $a_0 = 2.931$, $h = 6.908$, $\Delta = 1.629$, $\Delta_{soc} = 1.628$, $C_{11} - C_{12} = 326.239$, $e_{11} = 2.712$, $d_{11} = 0.831$
- **ZrSi$_2$N$_4**: $a_0 = 3.032$, $h = 7.035$, $\Delta = 1.629$, $\Delta_{soc} = 1.625$, $C_{11} - C_{12} = 287.008$, $e_{11} = 2.229$, $d_{11} = 0.777$
- **HfSi$_2$N$_4**: $a_0 = 3.022$, $h = 7.000$, $\Delta = 1.802$, $\Delta_{soc} = 1.789$, $C_{11} - C_{12} = 303.898$, $e_{11} = 4.442$, $d_{11} = 1.241$
- **CrSi$_2$N$_4**: $a_0 = 2.844$, $h = 6.869$, $\Delta = 0.498$, $\Delta_{soc} = 0.499$, $C_{11} - C_{12} = 358.021$, $e_{11} = 4.398$, $d_{11} = 1.145$
- **MoSi$_2$N$_4**: $a_0 = 2.909$, $h = 7.004$, $\Delta = 1.747$, $\Delta_{soc} = 1.746$, $C_{11} - C_{12} = 383.982$, $e_{11} = 4.398$, $d_{11} = 1.145$
- **WSi$_2$N$_4**: $a_0 = 2.912$, $h = 7.014$, $\Delta = 2.083$, $\Delta_{soc} = 2.074$, $C_{11} - C_{12} = 403.227$, $e_{11} = 3.138$, $d_{11} = 0.778$

Due to hexagonal symmetry, the two independent elastic stiffness coefficients ($C_{11}$ and $C_{12}$) are calculated by SSR, and all calculated elastic coefficients satisfy the Born stability criteria [27]. The elastic stiffness coefficients ($C_{11}$, $C_{12}$ and $C_{11} - C_{12}$) are shown in fig. 3. These elastic constants are larger than the ones of most 2D materials, like TMD, metal oxides, and III-V semiconductor materials [11,13], indicating that these 2D monolayers are more rigid than other 2D materials. The piezoelectric stress coefficients $e_{11}$ of the MSi$_2$N$_4$ monolayer are calculated by DFPT, using the rectangle supercell. Based on eq. (6), the piezoelectric strain coefficients $d_{11}$ are attained. The piezoelectric coefficients $e_{11}$ and $d_{11}$, and the ionic contribution and electronic contribution to $e_{11}$ are plotted in fig. 3. Some key data are also listed in table 1. For all six monolayers, it is clearly seen that the contribution to $e_{11}$ between ionic and electronic parts is opposite. The entire range of calculated $e_{11}$ is from 2.229 $10^{-10}$ C/m to 4.442 $10^{-10}$ C/m, while the $d_{11}$ ranges from 0.777 pm/V to 1.241 pm/V. Their $d_{11}$ are smaller than the ones of TMD monolayers (2.12 pm/V to 13.45 pm/V) [11,13]. For example, the $e_{11}$ of CrSi$_2$N$_4$ (4.442 $10^{-10}$ C/m) and MoSi$_2$N$_4$ (4.398 $10^{-10}$ C/m) are larger than the one of MoS$_2$ (3.64 $10^{-10}$ C/m), but their $d_{11}$ (1.241 pm/V to 1.145 pm/V) are smaller than the one of MoS$_2$ (3.73 pm/V) [11,13], which is due to larger $C_{11} - C_{12}$. Among all studied six monolayers, the CrSi$_2$N$_4$ monolayer has the best $d_{11}$.

The $d_{11}$ of the MSi$_2$N$_4$ monolayer is very small, and strain engineering is proposed to enhance their piezoelectric properties, which has been proved to be a very effective way [7,17,18]. Experimentally, biaxial strain can be achieved by exploiting the thermal expansion mismatch [28]. Here, we use the experimentally synthesized MoSi$_2$N$_4$ as an example to study the strain effects on piezoelectric properties. Due to 6$m_2$ symmetry, biaxial strain cannot induce polarization, not like uniaxial strain. We only consider biaxial strain effects on the piezoelectric properties of MoSi$_2$N$_4$, and the elastic constants $C_{11} - C_{12}$, piezoelectric coefficients $e_{11}$ and $d_{11}$, and the ionic contribution and electronic contribution to $e_{11}$ of monolayer MoSi$_2$N$_4$ as a function of biaxial strain are
Fig. 3: For MSi$_2$N$_4$ (M = Ti, Zr, Hf, Cr, Mo and W): the elastic constants $C_{ij}$ (top), piezoelectric stress coefficients $e_{11}$ and the ionic contribution and electronic contribution to $e_{11}$ (middle), and piezoelectric strain coefficients $d_{11}$ (bottom).

plotted in fig. 4. When the strain varies from −4% to 4%, the $C_{11} - C_{12}$ decreases, and the $e_{11}$ increases, which gives rise to improved $d_{11}$ based on eq. (6). At 4% strain, the $d_{11}$ is 2.375 pm/V, which is more than twice as large as the unstrained one (1.145 pm/V). Similar biaxial strain-improved $d_{11}$ can be found in monolayer g-C$_3$N$_4$ and MoS$_2$ with the same point group [29]. It is found that both ionic contribution and electronic contribution to $e_{11}$ have positive influence to improve $d_{11}$ of monolayer MoSi$_2$N$_4$, which is different from monolayer g-C$_3$N$_4$ and MoS$_2$ [29].

At applied strain, the monolayer MoSi$_2$N$_4$ exhibits piezoelectricity, which should have a band gap. The gap

Fig. 4: For the experimentally achieved monolayer MoSi$_2$N$_4$, the elastic constants $C_{ij}$ (top), piezoelectric stress coefficients $e_{11}$ and the ionic contribution and electronic contribution to $e_{11}$ (middle), and piezoelectric strain coefficients $d_{11}$ (bottom) as a function of biaxial strain.

Fig. 5: For the experimentally achieved monolayer MoSi$_2$N$_4$, the GGA+SOC gap and spin-orbital splitting at $K$ point as a function of biaxial strain.
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Fig. 6: For monolayers MoSi$_2$N$_4$, MoSi$_2$P$_4$, MoSi$_2$As$_4$ and MoGe$_2$N$_4$: the elastic constants $C_{ij}$ (top), piezoelectric stress coefficients $e_{11}$ and the ionic contribution and electronic contribution to $e_{11}$ (middle), and piezoelectric strain coefficients $d_{11}$ (bottom).

and spin-orbital splitting $\Delta$ at K point as a function of strain are plotted in fig. 5, and the strain-related energy bands of MoSi$_2$N$_4$ are plotted in fig. S3 of the SM. It is found that the gap decreases from 2.605 eV ($-4\%$) to 0.988 eV ($4\%$), while $\Delta$ increases from 0.122 eV to 0.134 eV. The position of conduction band minimum (CBM) does not change from $-4\%$ to 4\%, but the position of valence band maximum (VBM) changes from $K$ point to $\Gamma$ point. The valence bands convergence can be observed at about $-2\%$ strain due to almost the same energy between $K$ point and $\Gamma$ point, which is in favour of better p-type Seebeck coefficient. Similar strain-induced bands convergence can be observed in many 2D materials like PtSe$_2$ [30].

To further enhance piezoelectric properties, using elements of group IVA and elements of group VA to replace the Si and N elements in experimentally synthesized MoSi$_2$N$_4$, the monolayers MoSi$_2$P$_4$, MoSi$_2$As$_4$ and MoGe$_2$N$_4$ are proved to be stable [19]. The elastic constants $C_{11} - C_{12}$, piezoelectric coefficients $e_{11}$ and $d_{11}$, and the ionic contribution and electronic contribution to $e_{11}$ of monolayers MoSi$_2$N$_4$, MoSi$_2$P$_4$, MoSi$_2$As$_4$ and MoGe$_2$N$_4$ are plotted in fig. 6. It is clearly seen that monolayers MoSi$_2$P$_4$ and MoSi$_2$As$_4$ have a very higher $d_{11}$ than MoSi$_2$N$_4$, and they are 4.93 pm/V and 6.23 pm/V, which are comparable to one of most TMD monolayers [11]. One reason for the high $d_{11}$ for monolayers MoSi$_2$P$_4$ and MoSi$_2$As$_4$ is that monolayer MoSi$_2$P$_4$ and MoSi$_2$As$_4$ have more smaller $C_{11}$ and $C_{12}$ than MoSi$_2$N$_4$, which leads to smaller $C_{11} - C_{12}$. Another reason is that the minus of the ionic contribution to $e_{11}$ of monolayer MoSi$_2$P$_4$ is very small, and the ionic contribution is positive for monolayer MoSi$_2$As$_4$. The $d_{11}$ of monolayer MoGe$_2$N$_4$ is 1.83 pm/V, which is close to the one of MoSi$_2$N$_4$. 

**Conclusion.** — Significant progress has been achieved in synthesizing monolayer MoSi$_2$N$_4$ with a non-centrosymmetric structure, which allows it to be piezoelectric. Here, the piezoelectric properties of monolayer MSi$_2$N$_4$ (M = Ti, Zr, Hf, Cr, Mo and W) are studied by using first-principles calculations. In the considered six materials, CrSi$_2$N$_4$ is predicted to have the best $d_{11}$ of 1.24 pm/V, and the second is 1.15 pm/V for experimentally synthesized MoSi$_2$N$_4$. It is found that strain engineering can improve $d_{11}$ of MoSi$_2$N$_4$, and the $d_{11}$ at 4\% biaxial strain can improve by 107\%. Compared to monolayer MSi$_2$N$_4$ (M = Ti, Zr, Hf, Cr, Mo and W), the monolayers MoSi$_2$P$_4$, MoSi$_2$As$_4$ and MoGe$_2$N$_4$ have more higher $d_{11}$, and the $d_{11}$ of MoSi$_2$As$_4$ is as high as 6.23 pm/V. Owing to the recent CVD growth in monolayer MoSi$_2$N$_4$, it is expected that these monolayers MA$_2$Z$_4$ (M = Ti, Zr, Hf, Cr, Mo or W; A = Si or Ge; and Z = N, P or As) may be put to a wide practical piezoelectric use in the future.

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**Data availability statement:** The data that support the findings of this study are available from the corresponding author upon reasonable request.
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