

Supplementary Materials for Nano-scale displacement sensing based on Van der Waals interaction

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I. Vertical transitions corresponding to Peak I and Peak II.

Peak I in Fig.4 (b) corresponds to a vertical transition from an initial state in VB to CBM. In Fig. S1 we plot out the orbital probability density distribution of the initial state and CBM. One can see that for three different stacking configurations, both the initial state and CBM show the bonding character of delocalized states in the interlayer region. Therefore their energy variations are almost the same. That is the reason that Peak I almost keeps constant corresponds to the displacement. Peak II in Fig.4 (b) corresponds to a vertical transition from VBM to a final state in CB. From Fig. S1 one can see that the final state contains the interlayer delocalized probability density and σ bonding character while VBM does not. Therefore E_{VBM} remains constant and E_{PeakII} changes remarkably with the energy of the final state.

II. Fitting E_{CBM} and E_{PeakII} with quadratic equation

Both E_{CBM} and E_{PeakII} follow the quadratic equation express as: $E = E_0 - \beta d_z^{-2}$. The values of E_0 and β are shown in Table S1. Here E_0 converges to the E_{CBM}/E_{PeakII} value of single layer BP. β is determined by the interlayer hopping

integral of interacting orbitals, which is proportional to the wave function overlap. The β value of E_{CBM} is larger than E_{PeakII} , suggesting the hopping integral of CBM is larger than the final state of peak II in CB. For both E_{CBM} and E_{PeakII} , β is independent for different stacking configurations, which suggests that the interlayer hopping integral does not change much for different stacking configurations. This might be due to the delocalized distribution of the interacting orbitals. The d_z^{-2} law is described in tight-binding theory in ref [W. A. Harrison, Electronic Structure and Properties of Solids (Freeman, San Francisco,1980)].

		E_{CBM}	E_{PeakII}	E_{gap}
BLBP	$E_0(\text{eV})$	-2.31	4.80	3.4
	$\beta(\text{eV} \times \text{\AA}^2)$	18.0	11.5	18.0
Bi-layer MoS ₂	$E_0(\text{eV})$			3.0
	$\beta(\text{eV} \times \text{\AA}^2)$			10.5

Table S1. The values of E_0 and β for E_{CBM} and E_{PeakII} .

III. The electronic structure dependence on interlayer twisting.

The electronic structure of BLBP is also sensitive to the interlayer twisting. We have investigated the band gap change for the A-A stacking when the top layer is twisted around z axis shown in Fig.S2. The band gap varies from 1.75 eV to 2.34 eV when the twist angle θ changes from 0° to 180° . The total energy is within 13 meV. The interlayer distance d_z changes from 3.22 Å to 4.12 Å. The lowest energy configuration corresponding to $\theta=0^\circ$ has the smallest d_z , in which the CBM is stabilized to the lowest energy because of its σ bonding character.

The absorption intensity of different twisting angle is also investigated. The absorption intensity for A-A stacking BLBP with different interlayer twist angle is shown in Fig.S3 (a). The lowest two peaks corresponding to two direct excitation involves CBM and VBM as shown in Fig.S3 (b). Peak I corresponding to the vertical excitation to CBM does not change with the twist angle. Peak II corresponding to the vertical excitation from VBM changes from 3.65 eV to 4.18 eV when θ changes from 0° to 180° .

IV. Comparison with bi-layer MoS₂ and black phosphorus

We have compared BLBP with other corrugated bi-layer materials MoS₂ and black phosphorus. Fig. S4 shows the top view and side view of different stacking configurations of MoS₂ and black phosphorus. One can see that MoS₂ has similar structure with blue phosphorus (Fig. S4 (a)), which belongs to the graphene-like structures. As shown in Fig.5, similar with BLBP, E_{gap} of bi-layer MoS₂ can be fitted with $E = E_0 - \beta d_z^{-2}$. In contrast, the corrugation of black phosphorus is very large as shown in Fig. S4 (b), therefore the unified

$E_{gap} \propto dz^{-2}$ trend for different stacking configuration fails.

V. The effects of temperature

In order to convince the sensor works well in room temperature, we have performed ab-initio molecular dynamics investigation on BLBP with different stacking configurations. All the simulations are performed using VASP code.

We extended our unit cell to (5×5) . A time step of 1fs within a NVT ensemble was used. The system was equilibrated with a target temperature of 100K, 200K, 300K and 400K during 2ps. During all these molecular dynamics simulations, we did not find distinct change of the bi-layer atomic structure. As an example, we took snapshots every 100 fs in the molecular dynamics simulation at 300K and showed the interlayer distance d_z and band gap E_{gap} in Fig. S5 (a). We found that for all the three stacking configurations, d_z increases slightly when the temperature increases and it reaches the thermal equilibrium after 700 fs approximately. In order to test the d_z^{-2} law at different temperature, we obtained the d_z and E_{gap} for different temperatures after the systems reached thermal equilibrium. We found that d_z and E_{gap} at the temperature from 0 K ~ 400K for the 3 stacking configurations still follow the d_z^{-2} law as shown in Fig.S5 (b). Therefore we believe that the temperature does not affect the displacement measurement strongly.

VI. The test of strain effects

During the measurements, pulling one layer can be compensated by a local elastic deformation such as stretching or bending that restores the minimum energy stacking on some area. In order to test that possibility, we have calculated the elastic properties of BLBP. The biaxial strain can be imposed on BP layers by changing the lattice parameters a and b equally as shown in Fig. S6. Our results show that BP can sustain a stress up to about 9 N/m (Fig. S6 (a)). That corresponding tensile strain limits is 18%. This predicted elastic strain limit is close to that found in other 2D materials such as graphene, MoS₂ and black phosphorus respectively,¹⁻³ suggesting that BP is highly flexible and may have potential applications in flexible display. Our calculation of the total energy change as a function of the applied strain indicates the stretching (Fig.S6 (b)) and bending are much more difficult than interlayer displacement.

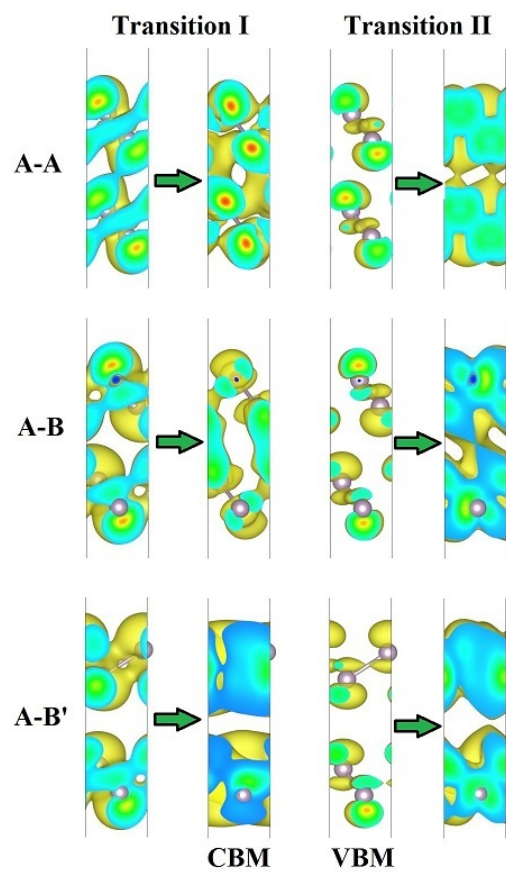


Fig. S1. The orbital probability density distributions of the initial and final states of vertical transitions corresponding to Peak I and Peak II for A-A, A-B and A-B' stacking BLBP.

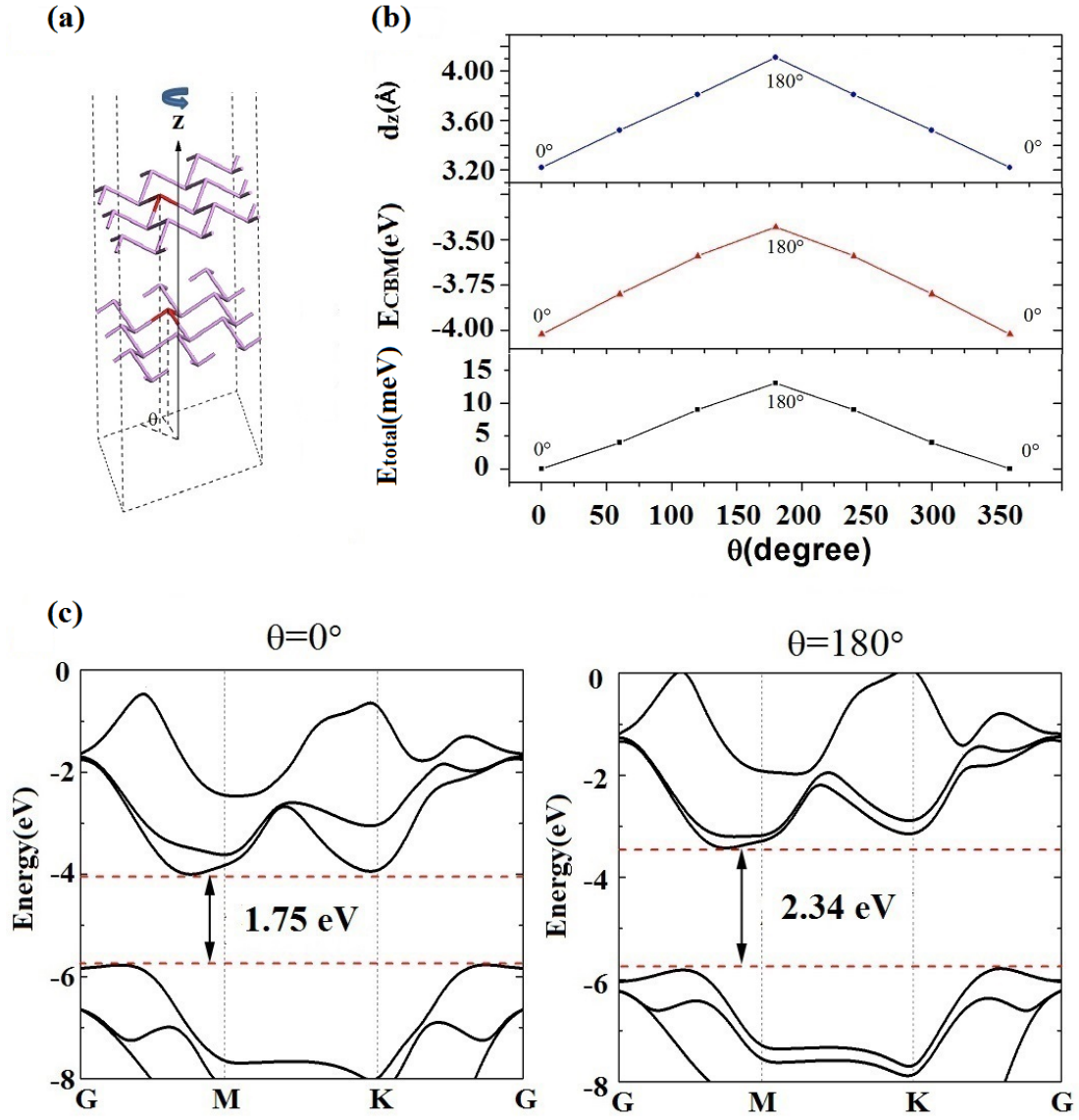


Fig. S2. The electronic structure dependence on interlayer twisting for A-A stacking BLBP. (a) The schematic diagram of interlayer twisting. (b) The change of E_{total} , E_{CBM} and d_z with twisting angle θ . (c) The plotting of band structure corresponding to $\theta = 0^\circ$ and $\theta = 180^\circ$.

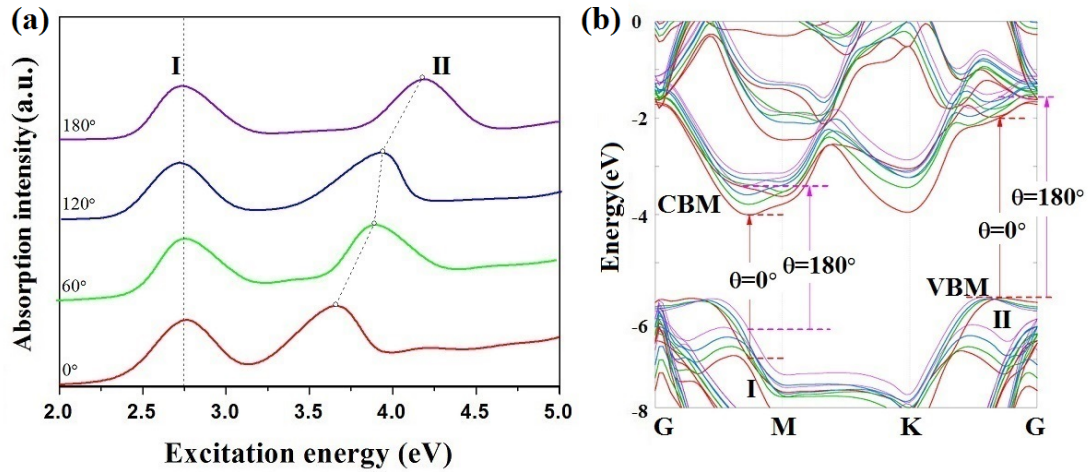


Fig. S3. The Absorption intensity (a) and band structure (b) of A-A stacking BLBP when the interlayer twisting angle θ changes from 0° (red line) to 180° (purple line). The two absorption peaks below 5 eV are marked as peaks I and II in (a). The corresponding vertical transitions for $\theta = 0^\circ$ and $\theta = 180^\circ$ are indicated by red and purple arrows in (b).

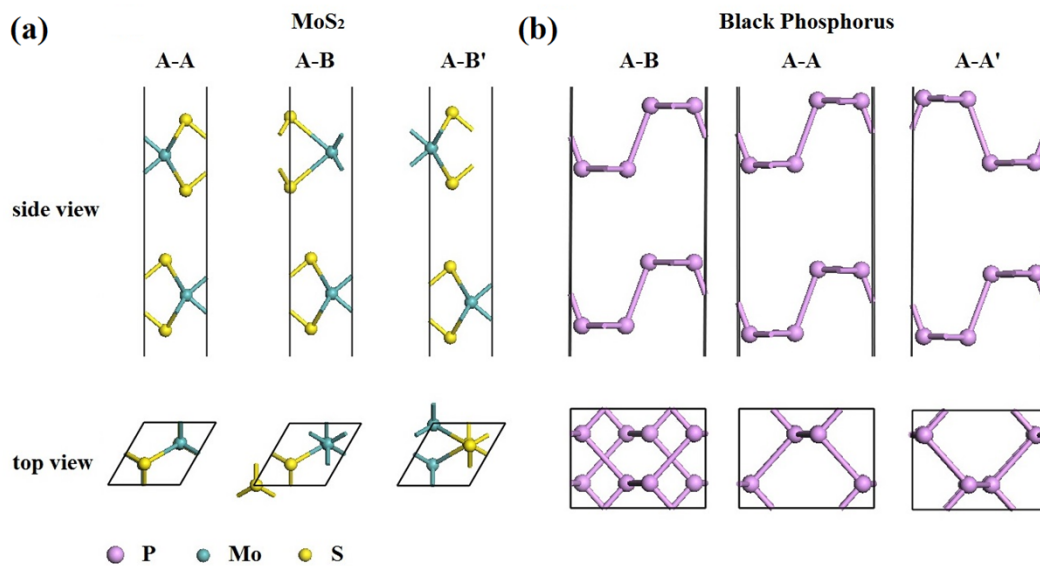


Fig. S4. The side view and top view of atomic structure of A-A, A-B, and A-B' stacking MoS₂ and black phosphorus.

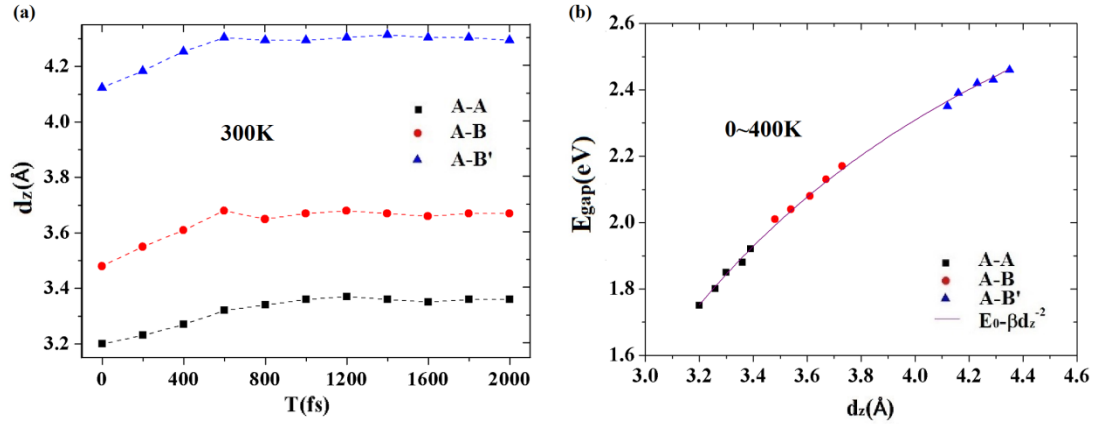


Fig. S5. (a) The change of d_z and E_{gap} during the molecular dynamics for A-A, A-B and A-B' stacking configurations with a target temperature of 300K. (b) The correlation of d_z and E_{gap} for different configurations at 0K, 100K, 200K, 300K and 400K.

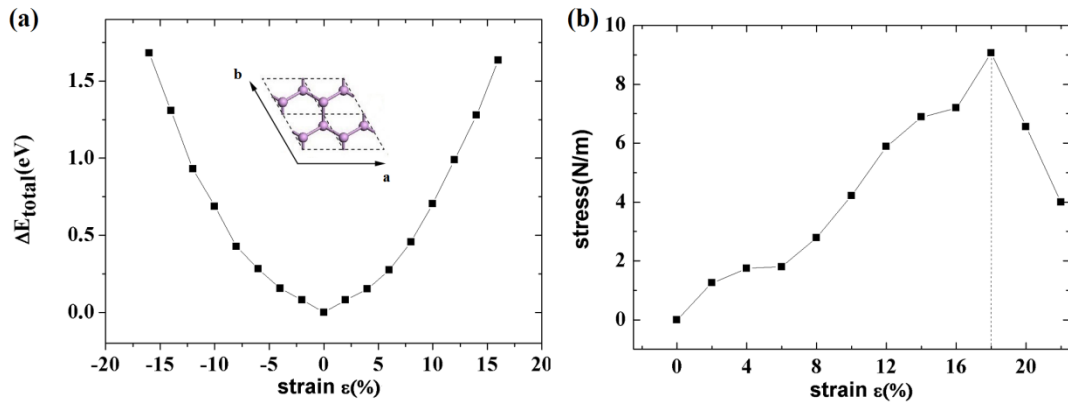


Fig. S6. (a) The stress as a function of tensile load for BP. (b) The change of total energy as a function of applied strain.

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