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Gate regulated near-infrared photodetector utilizing interlayer excitons for $MoS_2/CrPS_4$ heterojunction

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Excitons play an important role as interconnect in the optical and optoelectronic response and have attracted much attention for understanding the physical matters behind excitons [1, 2]. Excitons in atomically thin transition metal dichalcogenides semiconductors (TMDs) often trap an electron (X_-) or a hole (X_+) to form so-called trions, particularly in monolayers [3]. Though with exotic features and tunable bandgaps from visible to near-infrared (NIR) regions for TMDs, the issue of exciton physics in TMDs is inherently complex. It is already known that for bilayer TMDs (referred to homo-bilayers), interlayer coupling splits the degeneracy at the Γ point forming interlayer excitons (X_1), and the electronic transition transforms into an indirect gap semiconductor from the direct gap in monolayer [4]. This splitting is shown to be quite large even around 0.7 eV. Moreover, the rotational alignment of homo-bilayers or hetero-bilayers also influences the interlayer coupling in these bilayers from the previous experimental results [5]. Thus, TMDs and related van der Waals heterostructures (vdWHs) present an avenue for fundamental exciton physics because of their weak dielectric screening and strong geometrical confinement.

Principles of device design. The selection basis for making few-layer MoS_2-$CrPS_4$ (MS-CPS) vdWHs devices is introduced. Two reasons stand out prominently: (i) MoS_2 and $CrPS_4$ have different work functions forming type-II band alignment. (ii) MoS_2 and $CrPS_4$ have an approximate atomic arrangement, which produces a lattice mismatch variation. In the region of strong coupling, the electronic band structure and electron wavefunction are changed, which affects the tunneling processes of interlayer charge. So, the lattice mismatch in real space has a significant impact on the optical response for MS-CPS vdWHs. The structural information is directly probed using high resolution transmission electron microscopy (HRTEM). The electronic structure of the MS-CPS vdWHs is calculated by the density functional theory (DFT) method and the calculated indirect bandgap is ≈ 0.69 eV. In terms of the device architecture, we demonstrate a vertically integrated vdWHs photodetector composed of MoS_2 and $CrPS_4$. Then, the high performance of few-layer MS-CPS photodetectors from visible to NIR region has been realized. The electrode on top of the vertical heterojunction is the core part of the device because of the shorter carrier life of $CrPS_4$ about τ_{CrPS4} = 0.6 ns. This architecture guarantees the photoexcited electron-hole pairs generated from MS-CPS heterostructure in the vicinity of junctions can be extracted to the $CrPS_4$ electrode rapidly (Figure 1(a)). In particular, the heterojunction displays good gate-tunable modulation. The photodetector responds to near-infrared light of $\lambda = 1350$ nm with a photocurrent of 2.25 nA at $V_g = 5$ V and 8 pA at $V_g = -5$ V. And the cutoff wavelength is increased to 1500 nm with photocurrent of 150 pA at $V_g = 5$ V. This shows that the interlayer band gap shrinks under the control of the positive gate. Thus our findings exhibit a great probability for interlayer excitons applications.

Results and discussion. To calculate the band gap and prove if it has interlayer coupling in the MS-CPS heterojunction, we used DFT calculations and stacked the double layer MoS_2 and double layer $CrPS_4$ with the smallest interface strain. A large vacuum layer (38.16 Å) was chosen to avoid the interaction of the nearest heterojunctions. From the orbital resolved band structure, we found that the heterojunction has an indirect band gap of about 0.69 eV (Figure 1(b)). The electron could jump from the S 3p states to Mo 4d states. To see if the electrons jumped from $CrPS_4$ layer to MoS_2 layer, we projected the 3p states eigenstates of S in $CrPS_4$ nearby line 2, and 4d states of Mo in MoS_2 nearby line 1. The two eigenstates have an overlapping space between lines 1 and 2. So, the electrons of S 3p states in $CrPS_4$ layer could jump to Mo 4d states in MoS_2 layer across the overlapping space, indicating strong interlayer coupling and the probability of interlayer electronic transition in the MS-CPS heterojunction.

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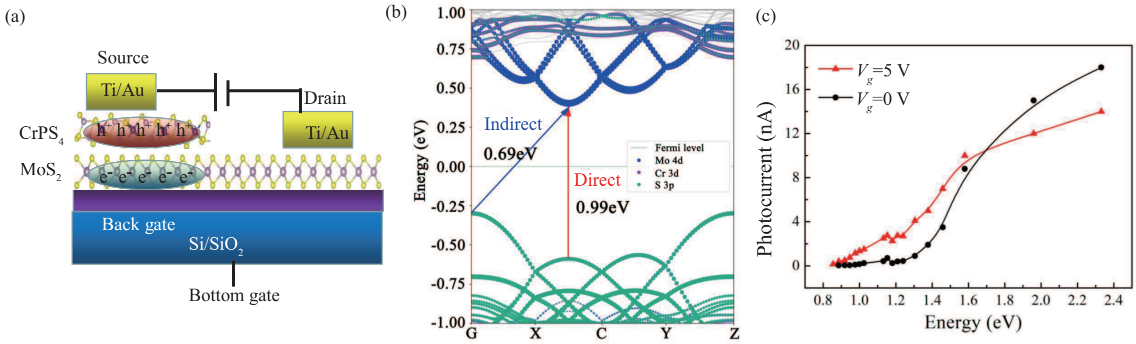

Figure 1 (Color online) (a) Schematic illustration of photodetector device; (b) the orbital resolved band structure by DFT method; (c) wavelength dependence of photocurrent for the MS-CPS photodetector.

To investigate the transport property, we measured the electrical performance of MS-CPS heterojunction. The interlayer photocurrent under the negative gate is too small to output steadily. Thus, we analyzed the photocurrent of this heterojunction device from 532 to 1500 nm wavelengths at $V_g = 0$ V and $V_g = 5$ V. As the excitation light wavelength increases, photocurrent decreases rapidly (Figure 1(c)). The photoexcited electron-hole pairs are separated by the applied electric field at the junction. The separated photoinduced holes and electrons generate current relating with intralayer excitons and interlayer excitons. Remarkably, there is a peak (about 0.7 nA at $V_g = 0$ V and 2.75 nA at $V_g = 5$ V) at round 1.15 eV with a larger photocurrent called valley current, corresponding to tightly bounded interlayer excitons. When photo excitation is beyond intrinsic transition, electron-hole bound pairs (excitons) are generated in MoS_2 and $CrPS_4$ interface layers. Then, the electrons in VBM of $CrPS_4$ transfer to CBM of MoS_2 forming interlayer excitons. Finally, owing to the type-II band alignment of the heterostructure, the photoexcited electrons and holes relax to the CB edge of MoS_2 and the VB edge of $CrPS_4$, respectively, via the interlayer relaxation process under forward bias. That is to say, interlayer excitons current is generated through the spatially indirect separation of the interlayer excitons. When a positive gate bias is applied, the energy band edges of both MoS_2 and $CrPS_4$ shift down. The electric field at the junction interface becomes smaller and more electrons transfer from $CrPS_4$ to MoS_2 to form excitons. Thereby a greater number of the photocarriers are generated at the interface. Then, more electron-hole pairs transfer from MoS_2 to $CrPS_4$ by exciton diffusion under external source electric fields. In contrast, the up-shifted MS-CPS energy band due to a negative gate bias increases the electric field at the junction interface so that the collection probability of photocarriers is reduced. Besides enhancing interlayer photocurrent, applying a positive gate extends wavelength response. The photocurrent response is expanded to 1500 nm wavelength with a smaller photocurrent of about 150 pA. In MS-CPS heterojunction, MoS_2 is on the bottom. Thus the positive back gate has a greater impact on the shift of Fermi level with MoS_2 compared with $CrPS_4$. This may induce that the energy interval in the heterojunction area was shrunk by a positive gate leading to excitons with lower energy producing photocurrent. Therefore, through the above analysis, the interlayer photoresponse characteristic is related to the region controlled by the gate bias, where the band offset and band bending in the type-II band alignment of the heterostructure are modulated.

Conclusion. We have demonstrated a highly efficient visible-NIR photodetector based on the interlayer optical transition. Indirect interlayer transitions can occur proved by DFT calculations. In particular, the exciton current is tuned by an external gate field and the cutoff wavelength is increased to 1500 nm. Remarkably, there is a peak of about 2.75 nA at $V_g = 5$ V around 1075 nm wavelength. Finally, this study on utilizing interlayer excitons for spatially separated electrons and holes in different layers is expected to offer a novel binary and ternary heterojunction device to overcome the limitation of the intrinsic band for high-performance NIR photodetectors.

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Supporting information Appendix A. The supporting information is available online at info.scichina.com and link.springer.com. The supporting materials are published as submitted, without typesetting or editing. The responsibility for scientific accuracy and content remains entirely with the authors.

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