High performance few-layer GaS photodetector and its unique red light photo-response in different gas environment

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Experimental section

Mechanical Exfoliation of GaS: Few-layer GaS nanosheet was isolated from bulk GaS single crystals and then deposited onto the freshly cleaned Si substrates covered by a 300 nm thick SiO_2 layer using the scotch tape-based mechanical exfoliation method, which was widely employed for preparation of single-layer graphene sheets.

Thermal Annealing: The samples were heated to 400 °C in a 25 °C/min rate and the temperature was held at 400 °C for one hour in vacuum. After annealing, the furnace was cooled down to room temperature and the samples were taken out of the furnace.

Photodetector devices were fabricated as follows: The Au electrodes were thermally evaporated by laying a Au wire with micrometer-sized diameter as the mask on GaS nanosheet exfoliated on the Si/SiO_2 substrates to obtain a gap between two electrodes. After the deposition of electrodes, the Au wire mask was removed so that the sample in gap area could be exposed. Photo-response experiments were all performed with a CHI660D electrochemical workstation in a conventional three-electrode electrochemical cell.

Raman Spectroscopy: Analysis of the few-layer GaS nanosheet by Raman spectroscopy was carried out on a WITec CRM200 confocal Raman microscopy system with the excitation line of 532 nm and an air-cooling charge-coupled device (CCD) as the detector (WITec Instruments Corp, Germany).

EDX analysis: EDX was utilized for the estimation the composition of GaS.

Density Functional Theory Calculations: The calculations were performed using

the projector augmented wave (PAW) method[1] with the generalized gradient approximation of Perdew-Burke-Ernzerhof (GGA-PBE)[2] exchange-correlation functional including van der Waals corrections[3], as implemented in the Vienna ab initio simulation package (VASP)[4]. Energy cutoff for plane-wave expansion was set to 500 eV. A large vacuum layer of 12 Å was adopted to avoid the interaction between adjacent images. Brillouin zone sampling was performed with Monkhorst Pack (MP) special k points meshes[5] including Γ point. K-points grids of was chose for the calculations with primitive unit cells, and was chose for the calculations with supercells. All the structures were fully relaxed using the conjugated gradient method until the Hellmann-Feynman force on each atom was less than 0.02 eV/Å. Bader analysis was used for the charge distribution on atoms[6].

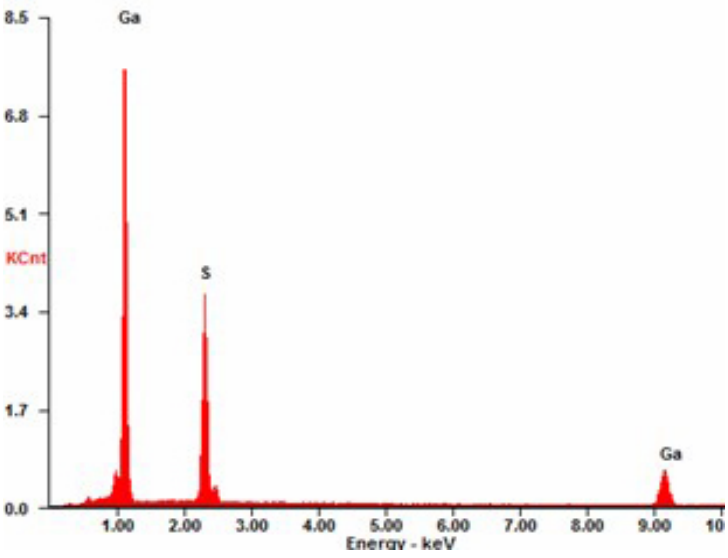

Figure S1 EDX of GaS nanosheet

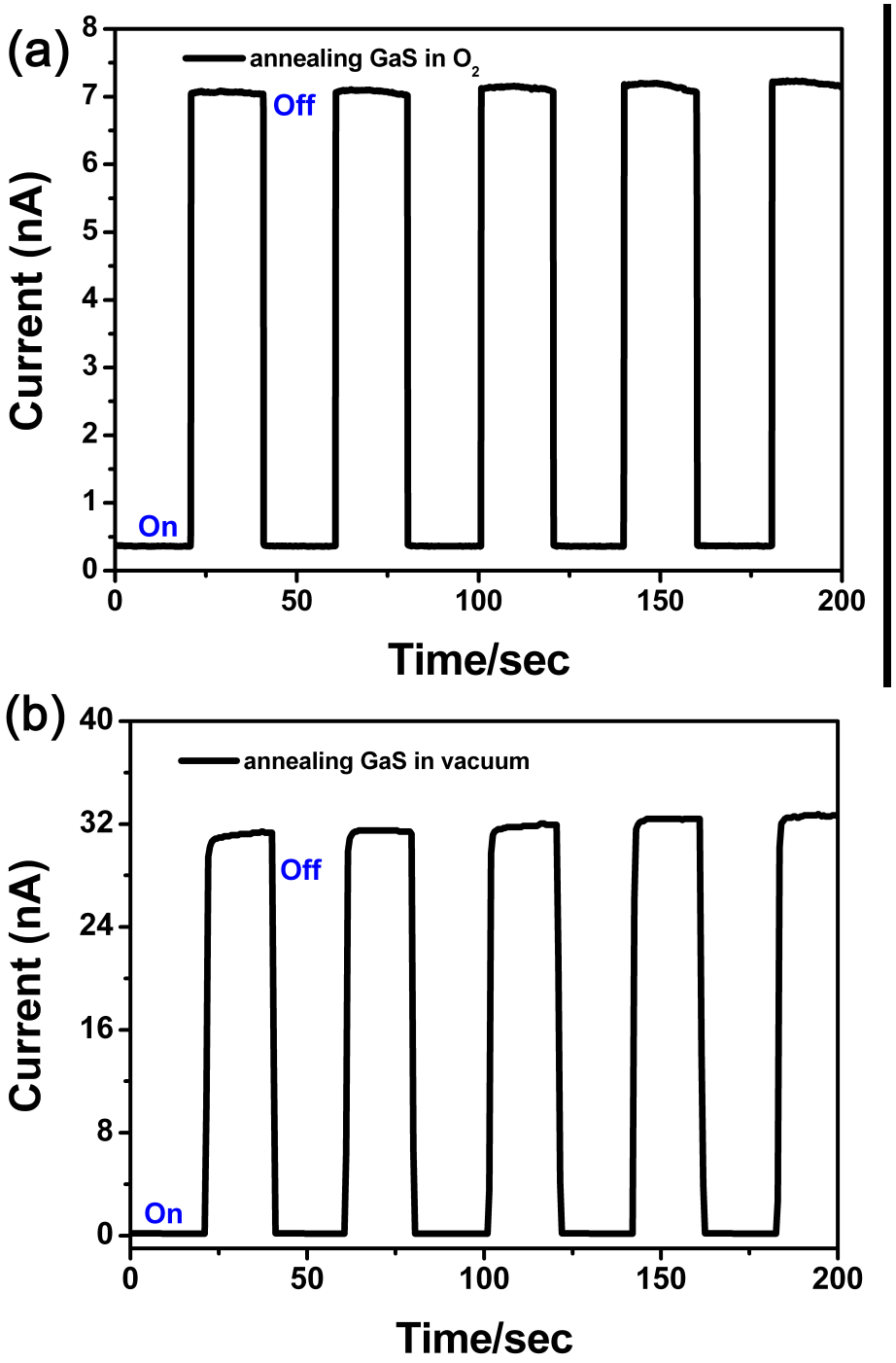

Figure S2 (a) I-t curve of the photodetector in O_2 gas environment and (b) I-t curve of the photodetector in vacuum.

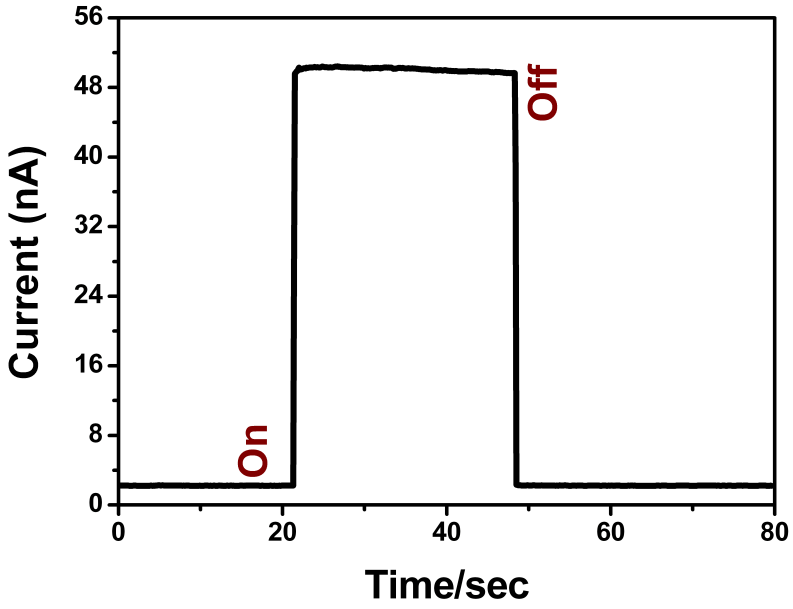

Figure S3 Saturated I-t curve of the photodetector in NH_3 gas environment.

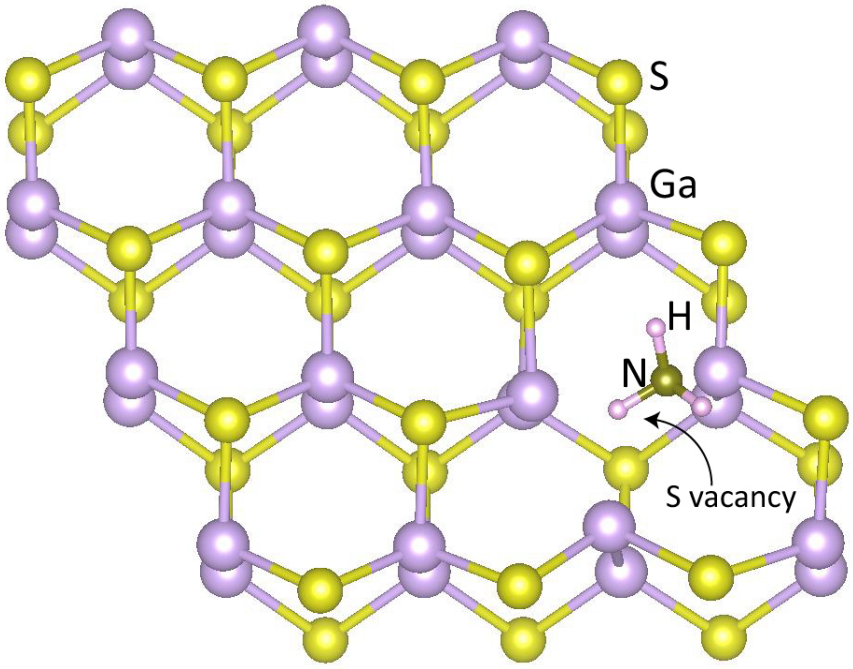

Figure S4 Adsorption of NH_3 molecule on monolayer GaS at the S vacancy site.

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