Supplementary Materials

Electrical tailoring of the photoluminescence of silicon-vacancy

centers in diamond/silicon heterojunctions

Xiaokun Guo ^{a,b}, Bing Yang ^{a,*}, Jiaqi Lu ^{a,b}, Haining Li ^{a,b}, Nan Huang ^a, LuSheng Liu ^a, Xin Jiang ^{a,c,*}

^a Shenyang National Laboratory for Materials Science, Institute of Metal Research (IMR), Chinese Academy of Sciences (CAS), No. 72 Wenhua Road, Shenyang, 110016, China

^b School of Materials Science and Engineering, University of Science and Technology of China, No. 72 Wenhua Road, Shenyang, 110016, China

^c Institute of Materials Engineering, University of Siegen, Paul-Bonatz-Str. 9-11, Siegen, 57076, Germany

*Corresponding author.

E-mail: byang@imr.ac.cn (Bing Yang), xjiang@imr.ac.cn (Xin Jiang).



Figure S1. The PL spectrum of the as-deposited diamond film excited by a 785 nm laser at liquid nitrogen temperature (77 K). A clear peak located at 948 nm indicates the presence of neutrally-charged SiV^0 centers. The inset shows the Raman spectra of the diamond film under the same excitation laser.



Figure S2. The SEM images of the diamond films annealed at various temperatures and durations: (a) 600°C-30 min; (b) 600 °C-60 min; (c) 700 °C-30 min.



Figure S3. XPS spectra of the C1 core carbon of the as-deposited samples before and after air annealing treatment: (a) the as-deposited sample; (b) the 600-30 sample; (c) the 600-60 sample; (d) the 700-30 sample. Due to the insulting nature of diamond, all the spectra are calibrated by aligning the sp³ C-C peak to the known literature value of 284.8 eV.



Figure S4. The PL spectra of the as-annealed sample before and after acid treatment. In this process, the as-annealed (600-30) sample was soaked in mixed acid (H_2SO_4 : $HNO_3 = 3:1$) at a temperature of 130°C for 120 min, in order to etch the surface sp²-C introduced in the annealing process. The PL result clearly shows that the surface graphitization plays a negligible role on the PL intensity of SiV⁻ centers in the whole depth.



Figure S5. The water contact angle of the as-deposited samples before and after air annealing treatment: (a) the as-deposited sample; (b) the 600-30 sample; (c) the 600-60 sample; (d) the 700-30 sample.



Figure S6. The PL signals collected at the region about 2 mm away from the electrodes with applying bias voltages on the diamond/ n^+ -Si heterojunction.



Figure S7. The PL spectra of the diamond/n⁺-Si heterojunctions at different forward bias voltages.



Figure S8. UPS valence band spectrum of the as-deposited H-terminated diamond film, exhibiting the energy difference from vacuum level (E_{VAC}) to valence band maximum (E_V) is estimated to 21.2 eV - 15.9 eV = 5.3 eV. The electron affinity of diamond (χ) was derived by: $\chi = E_{VAC} - E_C = E_{VAC} - E_V - E_g^{dia} = 5.3 - 5.47 = -0.17 eV$. All energies are measured relative to the common Fermi level that is determined from a reference gold foil.