Supplementary Materials for

Silicon nitride waveguides with directly grown WS_2 for efficient second-harmonic generation

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Fig. S1. Fundamental TE mode distribution of Si_3N_4 waveguide and silica fiber covered by a monolayer WS₂. (a) Fundamental TE mode distribution of the TE mode in the Si_3N_4/WS_2 hybrid waveguide structure. The width and the height of the Si_3N_4 waveguide is 2.0 µm and 0.6 µm, respectively. The thickness of the WS₂ monolayer is set to be 0.65 nm. (b) Fundamental TE mode distribution of a microfiber covered by a monolayer WS₂. The diameter of the core is set to be 4 µm.

We use the simulation software "*COMSOL*". The wavelength is set to be 1,550 nm and the refractive index n of monolayer WS_2 is set to be 4.5.¹ Fig. 1 shows the fundamental TE mode distribution of the Si_3N_4 waveguide covered by a monolayer WS_2 on the top and both sides and a 4 µm-diameter microfiber also covered by a monolayer WS_2 . The confinement factor of the monolayer WS_2 can be expressed as:²

$$\Gamma = \frac{\int_{ws_2} \varepsilon_{ws_2} |E_{\parallel}|^2 dV}{\int_{V} \varepsilon |E|^2 dV}$$

Where ε is the dielectric constant, and E_{\parallel} is the electric field in the analyzing plane. $\Gamma \approx 0.17\%$ for the Si₃N₄/WS₂ hybrid waveguide and $\Gamma \approx 0.065\%$ for the SiO₂/WS₂ microfiber. The confinement factor in the hybrid waveguide is 162% higher than that in the microfiber.

For the same pump power, we calculated the magnitude of electric field |E| in the monolayer WS₂ for the P₁ point in Fig. 1(a) and the P₂ point in Fig. 1(b). The results show that the value of |E| at P₁ is about 27 times as much as that of the point P₂, which means that the second-order nonlinearity of the Si₃N₄/WS₂ hybrid waveguide is much higher than that of the microfiber covered by a monolayer WS₂, since the SHG effect is proportional to $|E|^2$.



Fig. S2. SEM image of the Si_3N_4 waveguide with SiO_2 etched at both sides before the subsequent WS_2 growth.

References

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