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Strong coupling and catenary field enhancement in the hybrid plasmonic metamaterial cavity and TMDC Monolayers

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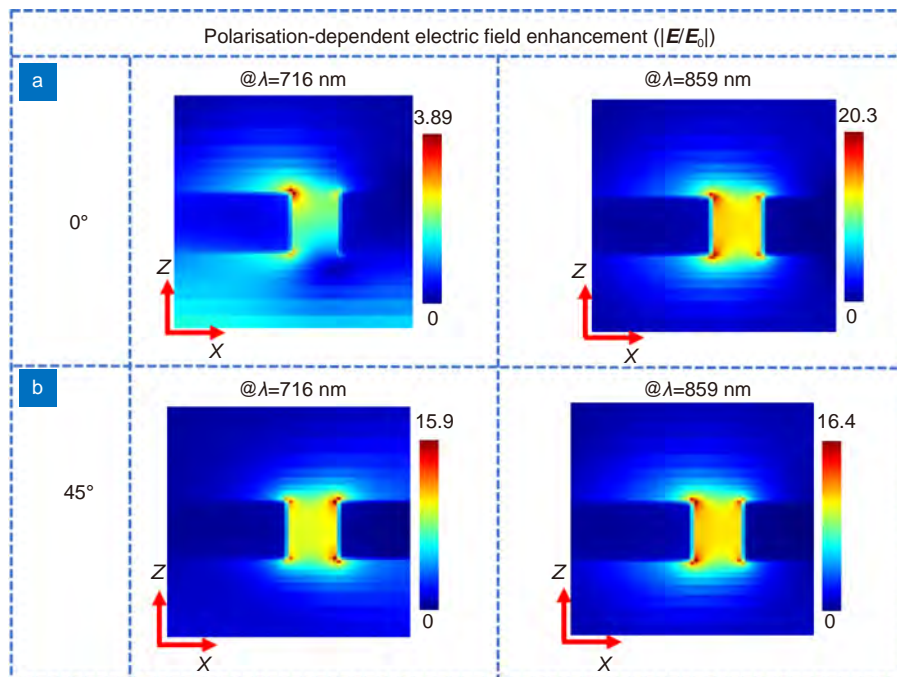


Fig. S1 | Polarization-dependent near-field enhancement. Electric field enhancement of the uncoupled Au cavity at a polarisation angle of (a) 0° and (b) 45° . The geometry of the Au cavity was the same as shown in Fig S1. (a).

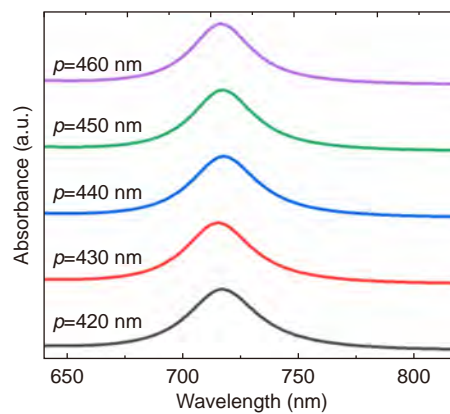


Fig. S2 | Effect of period on tuning plasmon resonance of uncoupled Au cavity. The plasmon resonance is not tunable with varying periods. The design parameters of the nanostructure are set as constants with $W_1 = 39$ nm, $W_2 = 33$ nm, $h = 157$ nm, $g = 108$ nm, $\alpha = 307$ nm, and $t = 60$ nm (see Fig. 1(a)).

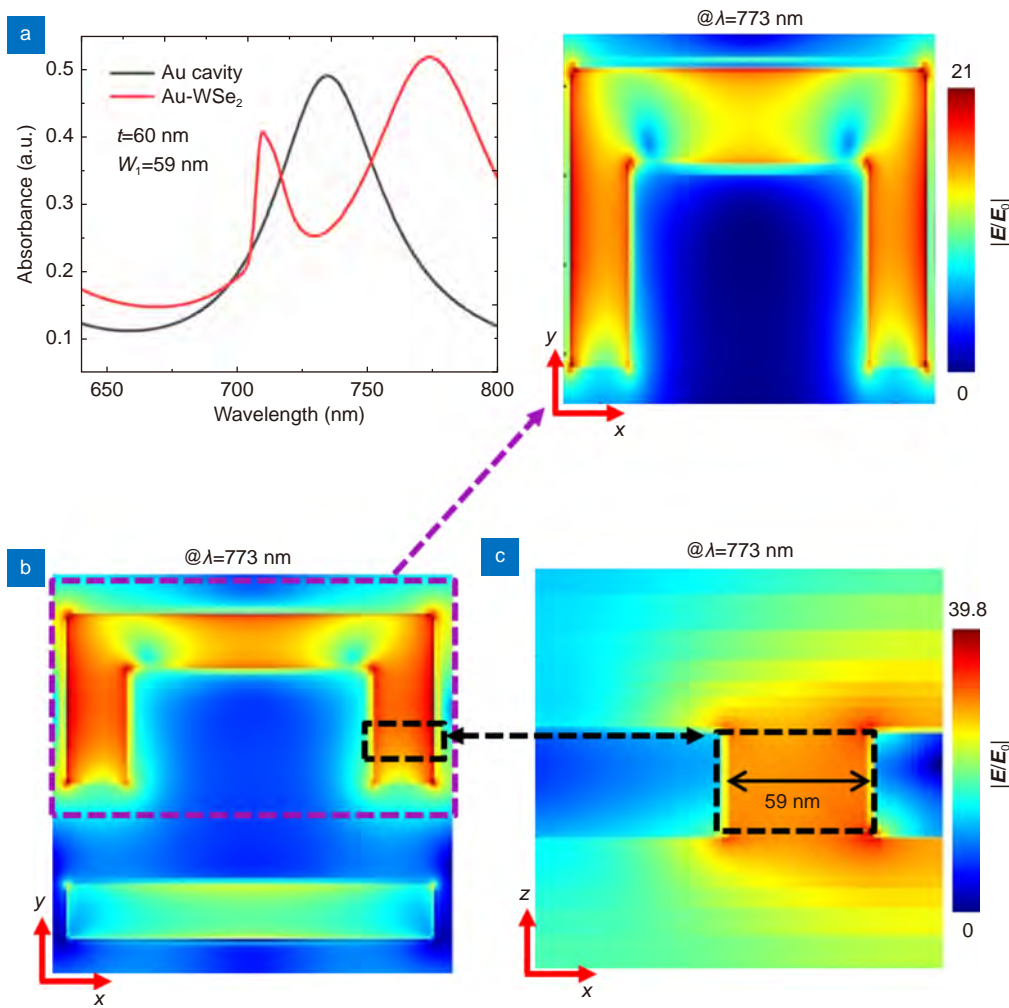


Fig. S3 | Effect of cavity gap on absorbance and near-field enhancement of Au-WSe₂. (a) Absorbance of Au-WSe₂, and the corresponding electric field generated at a unit cell of the Au cavity, for at the planes (b) $z = 13$ nm, and (c) $y = 70$ nm. In the Au-WSe₂ nanostructure, the design parameters of the Au structure are set follows: $W_1 = 59$ nm, $W_2 = 53$ nm, $h = 166.5$ nm, $g = 98$ nm, $\alpha = 327$ nm, and $t = 60$ nm.

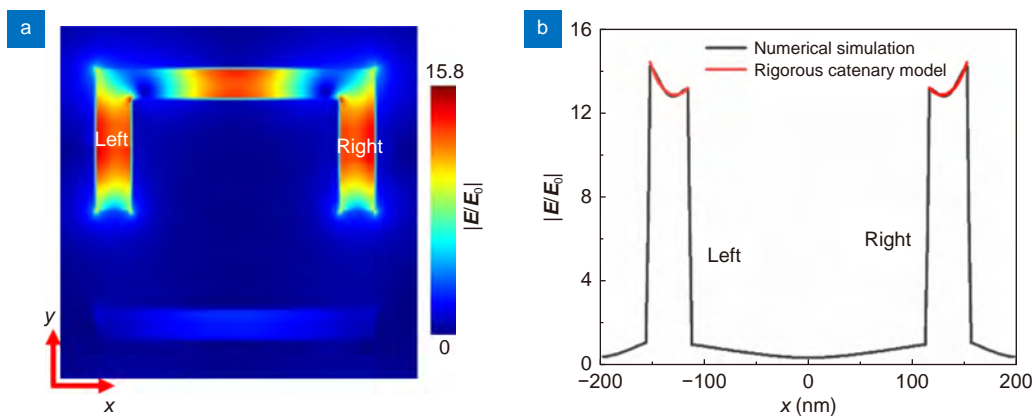


Fig. S4 | The modelled catenary-shaped near-field enhancement. (a) The electric field profile of Au cavity, at the z planes with a polarization along the y -axis. (b) The retrieved catenary-shaped near-field enhancement of uncoupled Au cavity. The extracted field distribution of the left- and right-sides are symmetric and are matched with the catenary model.

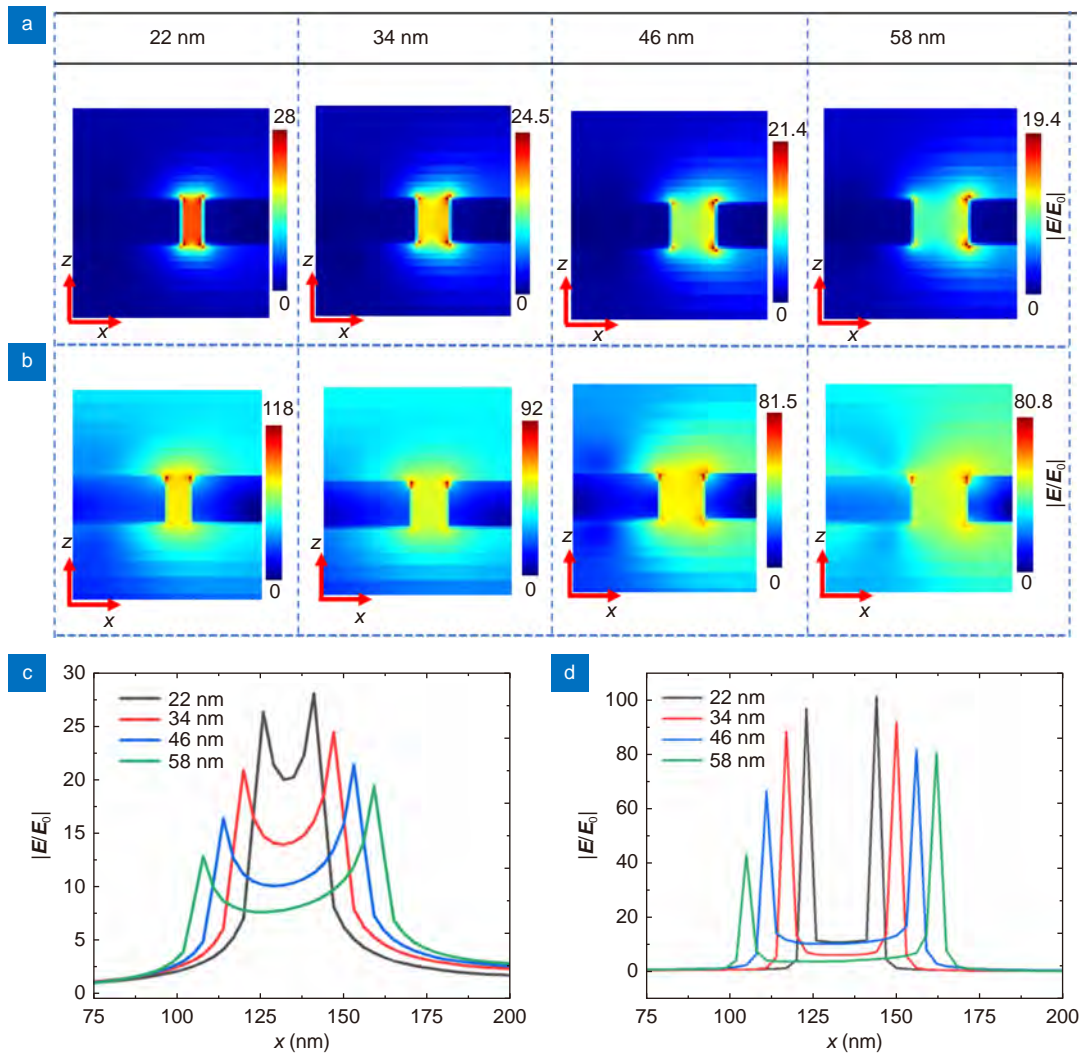


Fig. S5 | Electric field profile and their corresponding catenary-shaped near-field enhancement. Here, for the comparison of electric field profiles, the thickness of the Au cavity is set at 50 nm, while changing other parameters ($W_1 = 22\text{--}58$ nm, $W_2 = 16\text{--}52$ nm, $g = 98.5\text{--}116.5$ nm, $\alpha = 290\text{--}326$ nm, and $h = 148.5\text{--}166.5$ nm). Calculated near-field intensity distribution of (a) uncoupled Au cavity, and their corresponding (b) Au-WSe₂ heterostructure. The electric field profile revealed that the electric field confinement is enhanced in Au-WSe₂ heterostructure compared to uncoupled Au cavity has great implications to induce plasmon-excitons coupling. The electric field profile was captured at the resonance point. The extracted electric field distribution in (c) Au cavity, and (d) Au-WSe₂ heterostructure with varying cavity gaps. The catenary-shaped near-field enhancement revealed the plasmon coupling is strongly dependent on the cavity gap distance.

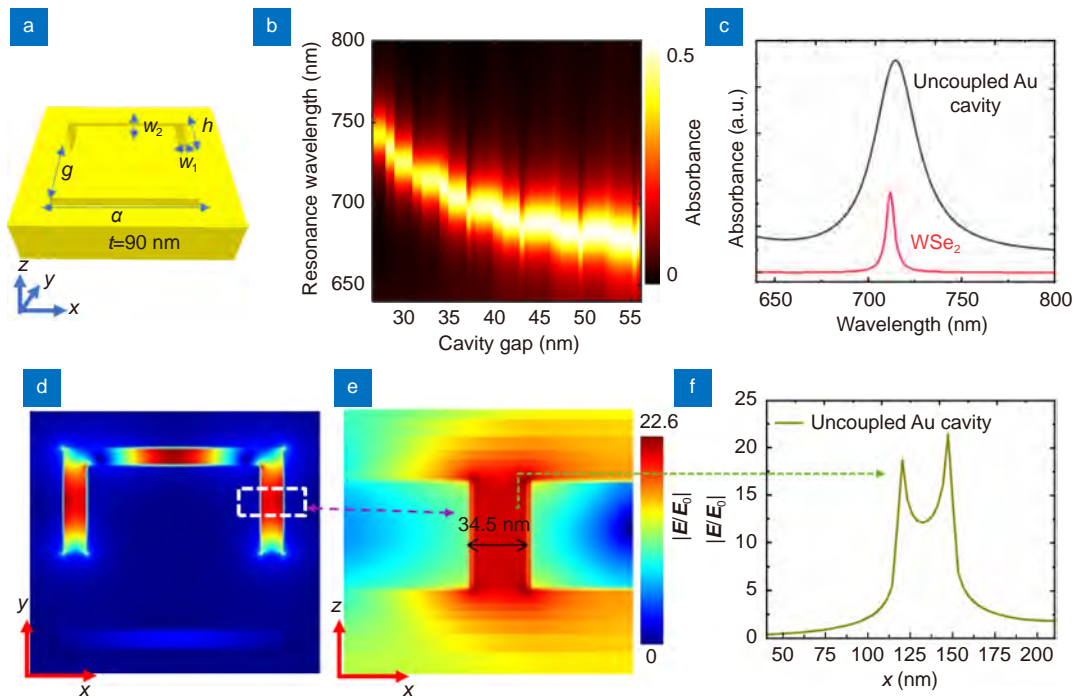


Fig. S6 | Effect of cavity gap on tuning Au plasmon resonances. (a) Schematic drawing of Au nanostructure with a thickness $t = 90$ nm and varying cavity gaps of W_1 from 22 to 58 nm and W_2 from 16 to 52 nm, while other parameters are kept the same as in Fig. 2(a). (b) Absorption mapping of Au cavity at a period of $p = 420$ nm. (c) The absorption spectra of Au cavity (black line) and the uncoupled WSe₂ monolayers (red line). The electric field generated at a unit cell of the Au cavity, at the planes (d) $z = 13$ nm, and (e) $y = 70$ nm with a polarization along the y -axis. (f) The retrieved catenary-shaped near-field enhancement at air-gold interfaces.

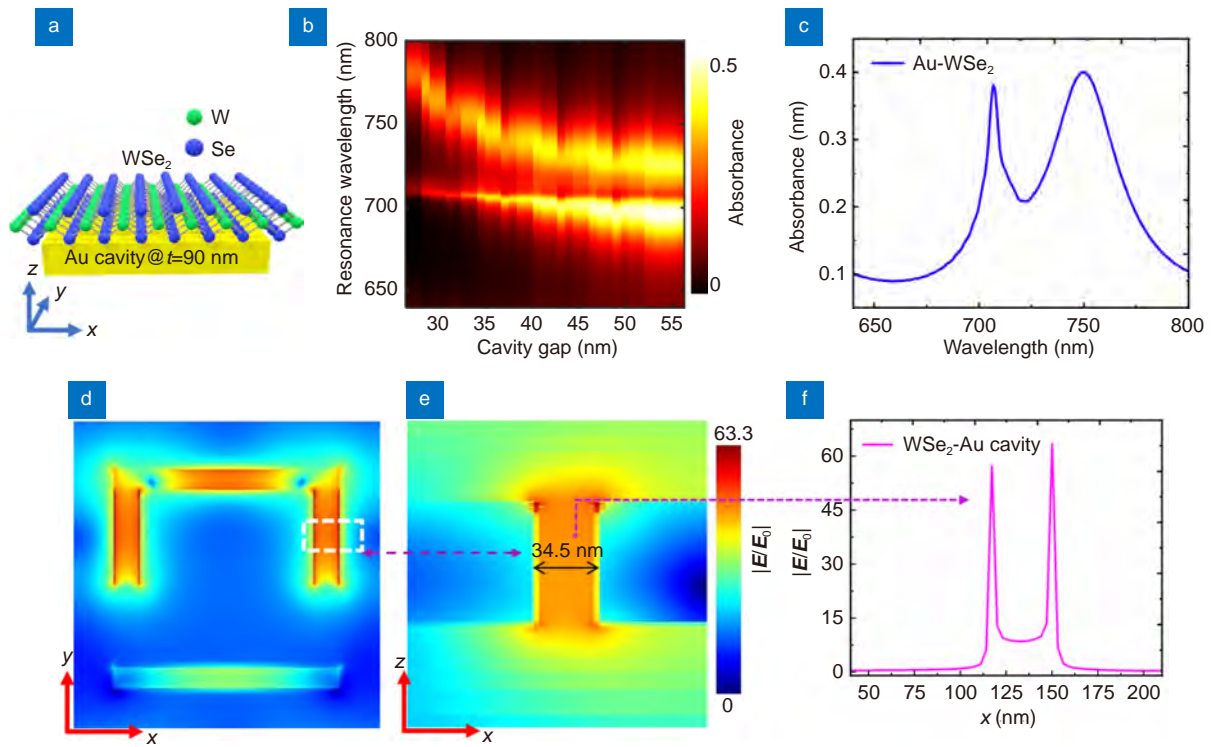


Fig. S7 | Effect of cavity gap on strong coupling of Au-WSe₂ heterostructure. (a) Schematic illustration of monolayer WSe₂ on top of Au cavity at normal incidence. (b) Absorption spectrum mapping of Au-WSe₂ as a function of cavity gap distance (W_1). (c) Absorption spectrum of Au-WSe₂ corresponding to figure (b) with a cavity gap of $W_1 = 34.5$ nm by $W_2 = 28.5$ nm. Electric field distribution at a unit cell of Au-WSe₂ nanostructure in the planes (d) y -plane and (e) z -plane taken at their resonance point. (f) The retrieved catenary-shaped symmetric electric field profile of Au-WSe₂.

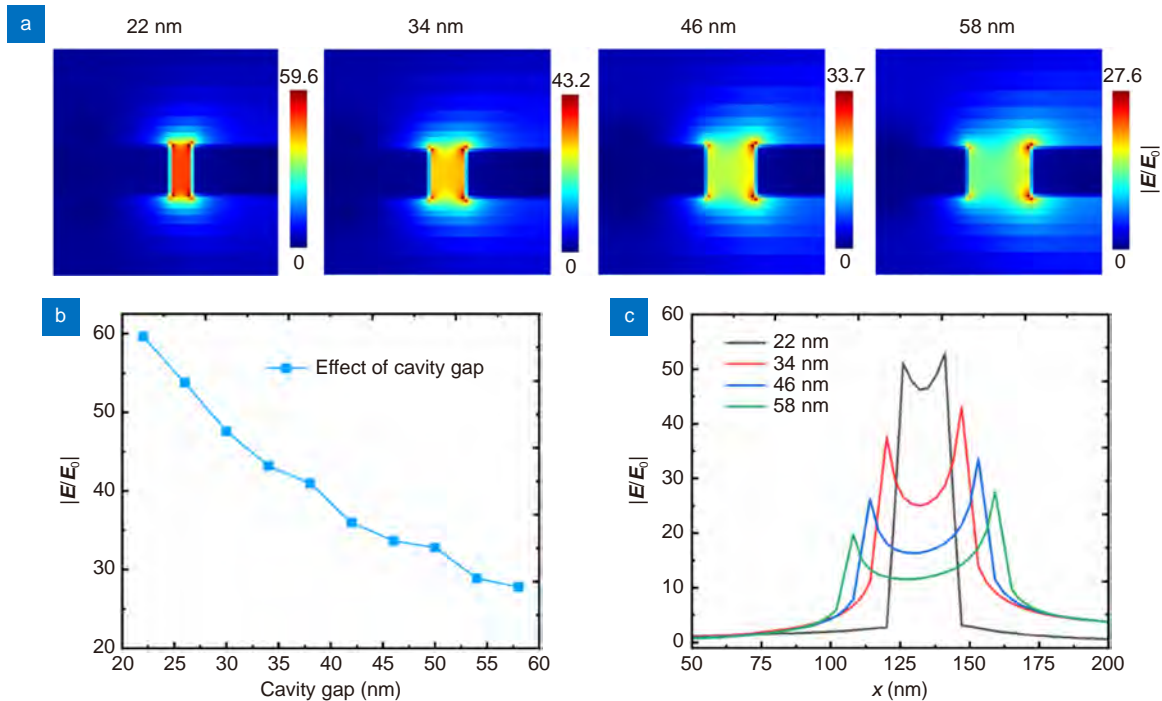


Fig. S8 | Catenary-shaped optical fields in a thin Ag cavity. The thickness of the Ag cavity is 50 nm and varying other parameters ($W_1 = 22$ –58 nm, $W_2 = 16$ –52 nm, $g = 98.5$ –116.5 nm, $a = 290$ –326 nm, and $h = 148.5$ –166.5 nm). (a) The electric field distributions of Ag cavities at their corresponding resonance frequency. (b) The magnitude of electric field induced in the cavity, which is corresponding to the results in (a). (c) Retrieved catenary-shaped near-field profile of (a).

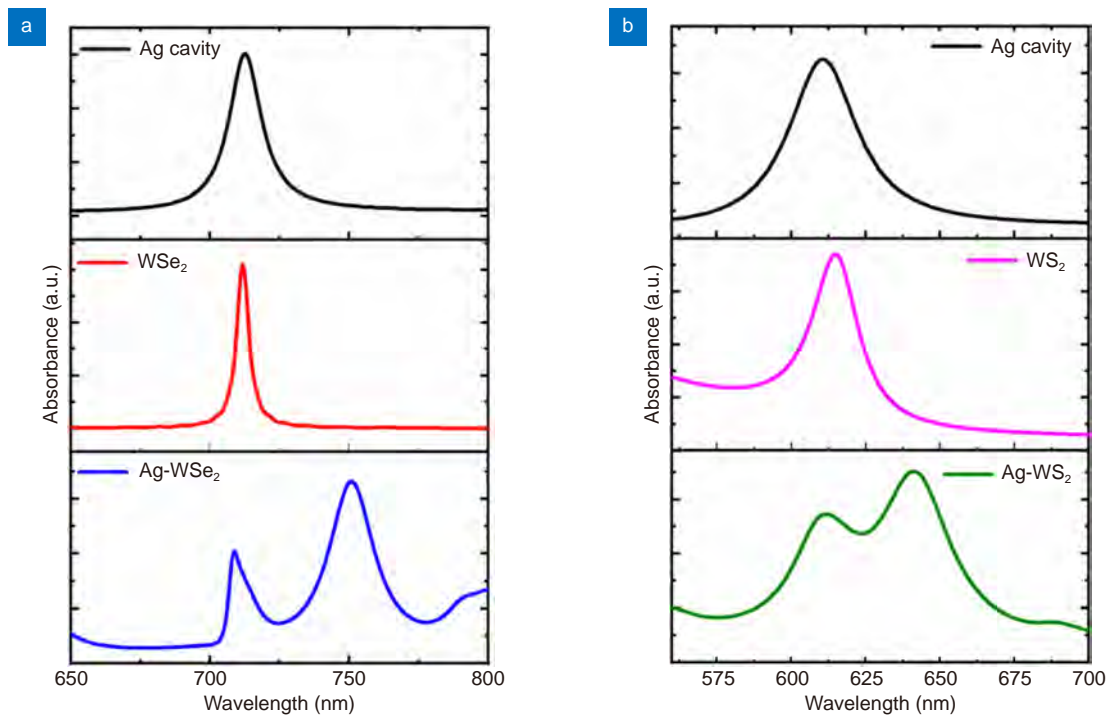


Fig. S9 | Strong coupling in the Ag-WSe₂ and Ag-WS₂ heterostructures. (a) Absorption spectra of the uncoupled Ag cavity (top), uncoupled WSe₂ monolayers (middle), and their Ag-WSe₂ hybrid nanostructure. The design parameters of Ag cavity were set as follows: $W_1 = 39$ nm, $W_2 = 33$ nm, $h = 157$ nm, $g = 108$ nm, $\alpha = 307$ nm, and $t = 50$ nm (see Fig. 2(a) for the position of the parameters). To align the plasmon resonance of Ag cavity with excitons of WSe₂, period was set at 560 nm. (b) Absorption spectra of uncoupled Ag cavity (top), uncoupled WS₂ monolayers (middle), and their Ag-WS₂ hybrid nanostructure. The design parameters of Ag cavity were set as follows: $W_1 = 70$ nm, $W_2 = 60$ nm, $h = 157$ nm, $g = 108$ nm, $\alpha = 307$ nm, and $t = 50$ nm (see Fig. 2(a) for the position of the parameters). To align the plasmon resonance of Au cavity with excitons of WSe₂, period was set at 430 nm. To note that the quality factor of (Q) of the Ag cavity can be enhanced by increasing the period (see Fig. 5(c)). In Ag-WSe₂ and Ag-WS₂ heterostructures, two absorption peaks are observed corresponding to the UPB and LPB.