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Supporting Information for Schottky barrier effect on plasmon-induced charge transfer

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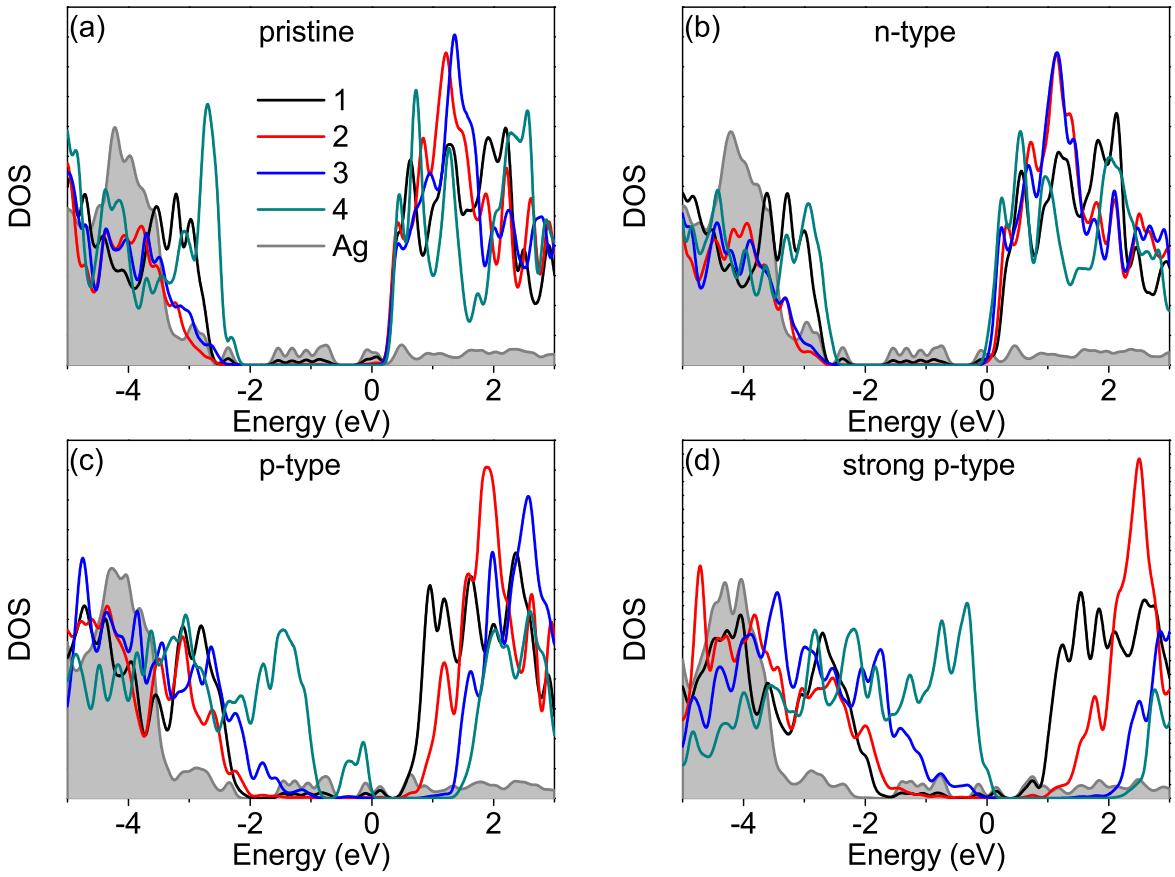

Figure S1: The local density of states of the four TiO_2 layers and the Ag nanocluster for the pristine (a), n-type (b), p-type (c) and strong p-type (d) systems, respectively.

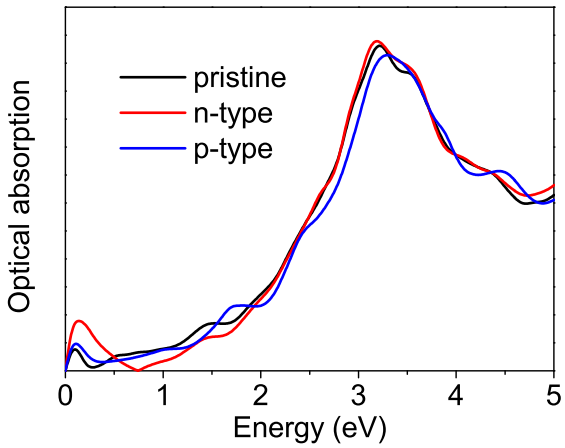

Figure S2: The optical absorption spectra for the pristine, n-type, and p-type systems, respectively. The plasmonic peak is at 3.2 eV. The doping in TiO_2 has negligible effect on the optical absorption.

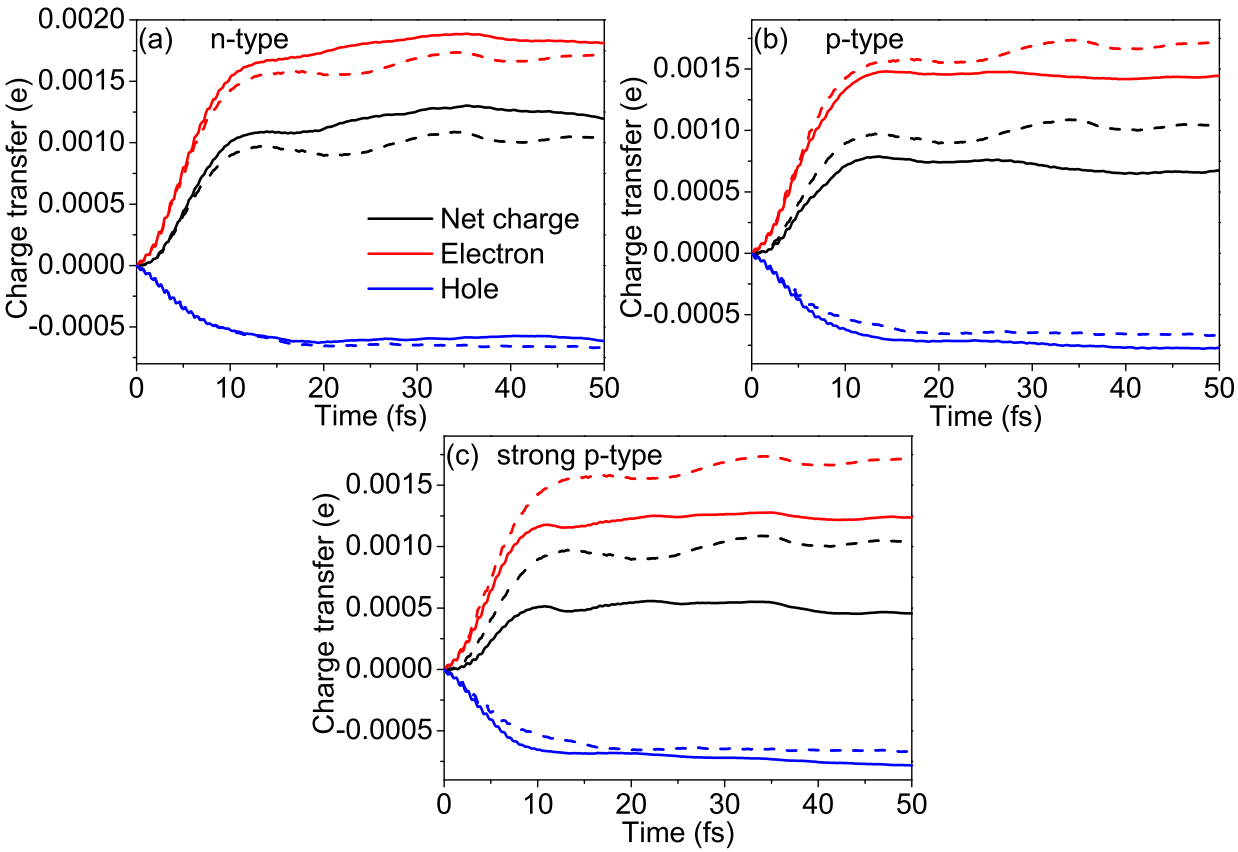

Figure S3: The electron transfer, hole transfer, and net charge transfer as a function of time for the n-type (a), p-type (b) and strong p-type (c) systems, respectively. The results for the pristine system are plotted as the dashed lines for comparison. According to our definition, the electron transfer is positive and the hole transfer is negative (i.e., the absolute value of the blue line gives the number of transferred hot holes).

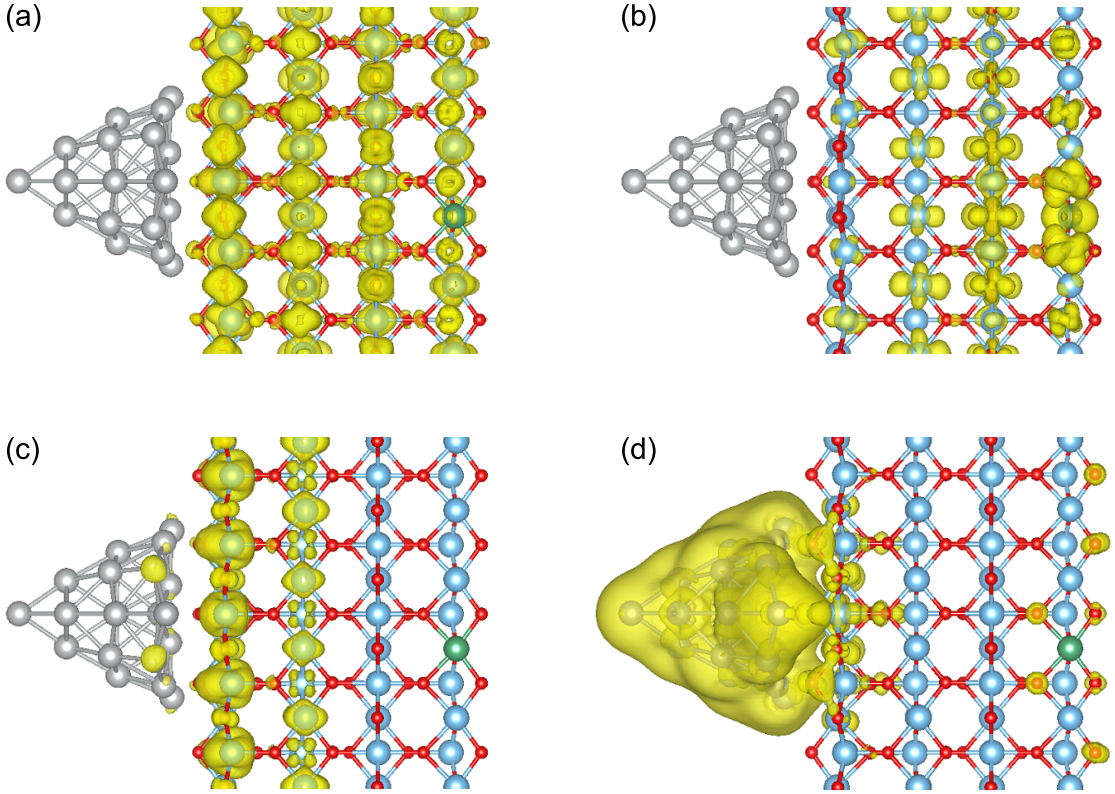

Figure S4: The charge densities for hot electrons in the band region (a) and the band bending region (b) of the n-type system. The charge densities for hot electrons (c) and hot holes (d) in the band bending region of the p-type system.

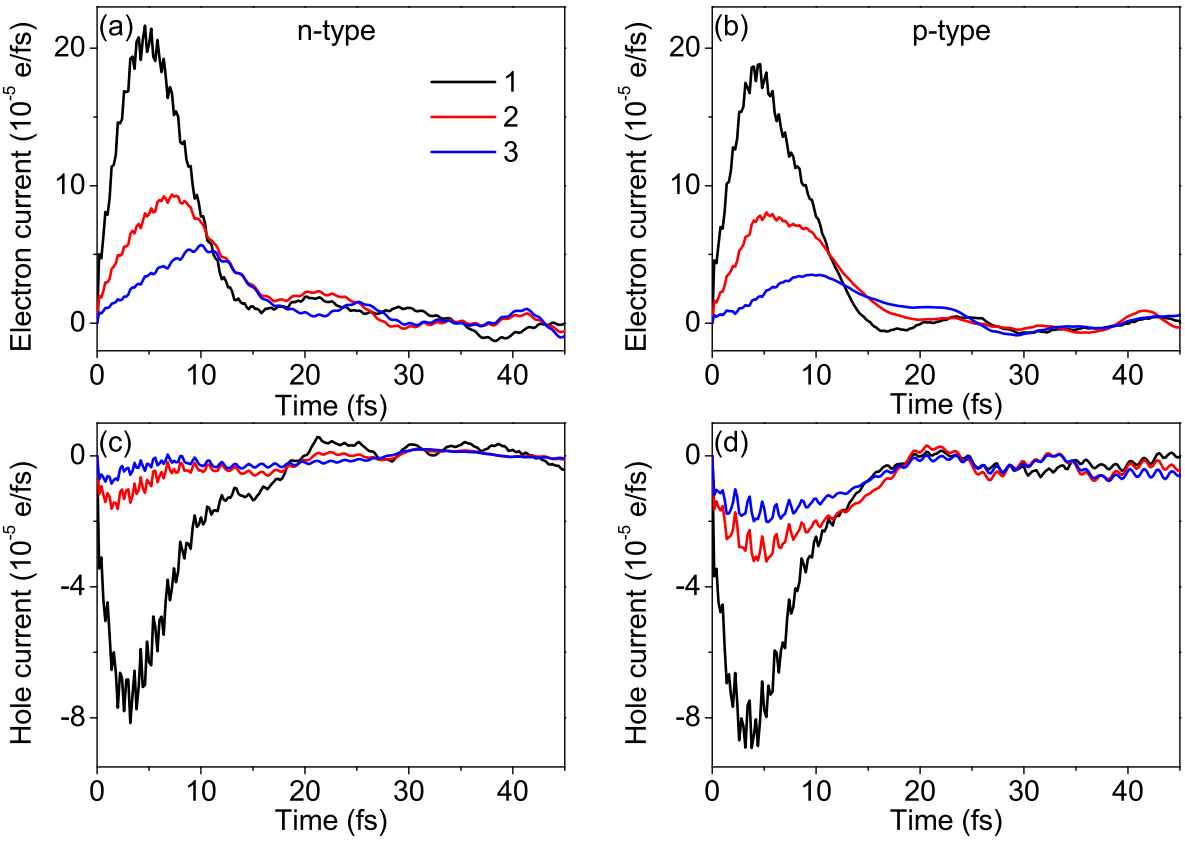

Figure S5: The electron currents and hole currents through the TiO_2 layers for the n-type system with the band bending of -0.2 eV (a, c) and the p-type system with the band bending of 1.1 eV (b, d). Because the fourth layer has the dopant, it is not shown.

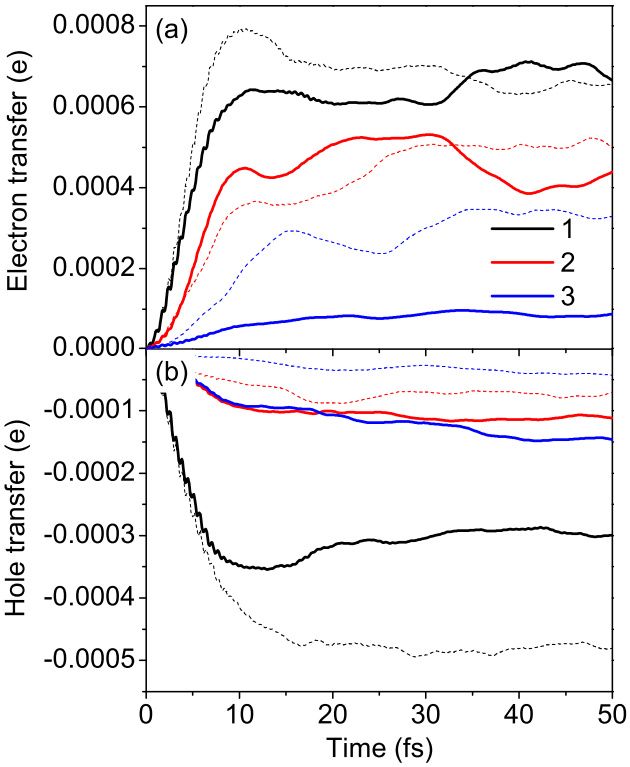

Figure S6: The electron transfer and hole transfer in every TiO_2 layer of the strong p-type system (solid lines). Because the fourth layer has the dopant, it is not shown. For comparison, the charge transfers of the pristine system are also shown (dashed lines).