Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

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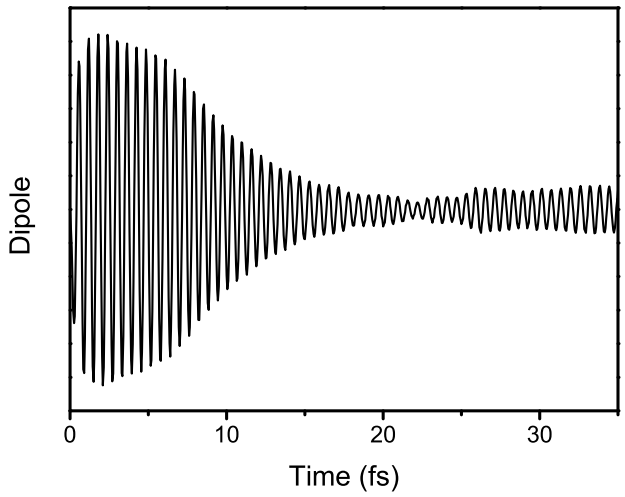

Figure S1: The dipole oscillation of the Al_{19}-TiO_2 system under the illumination of a 6.75 eV laser pulse. It decays within 15 fs, indicating the damping of the plasmon.

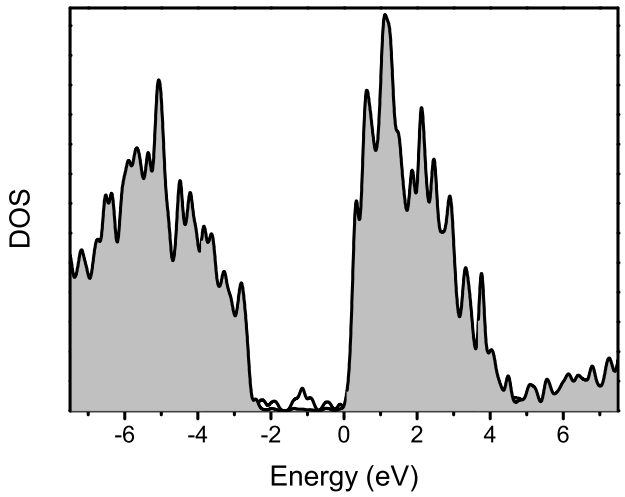

Figure S2: The density of states of the Al_{19}-TiO_2 system. The Fermi level is at 0 eV. The grey regions represent the TiO_2 valence bands and conduction bands. The mid gap states are derived from the Al_{19} nanocluster.

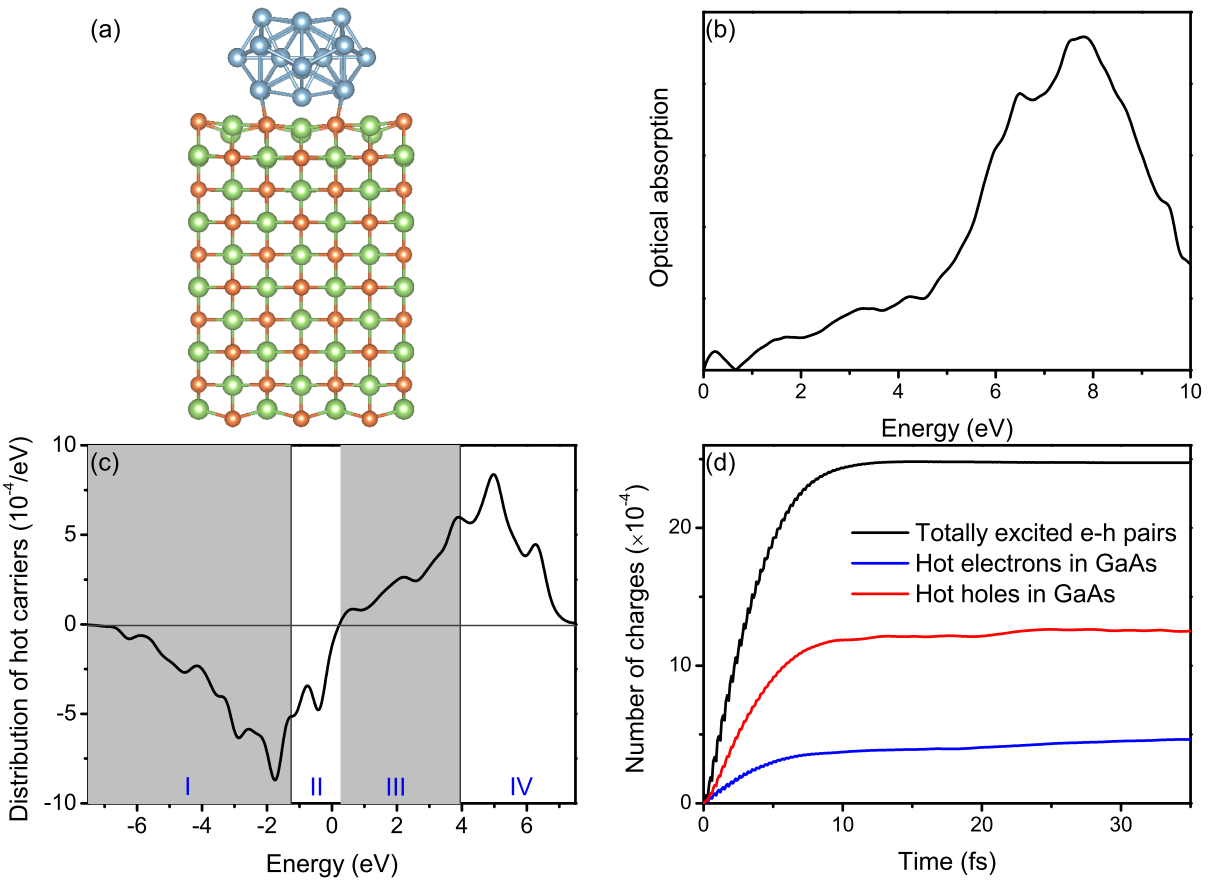

Figure S3: The optimized structure (a), the optical absorption spectrum (b), the hot carrier distribution at 30 fs (c), and the numbers of totally excited electron-hole pairs, hot holes and hot electrons in the GaAs (d) for the Al_{19}-GaAs system. The excitation frequency is 6.75 eV. In the calculations, the electronic structure of GaAs has been corrected to reproduce the experimental band gap and electron affinity.

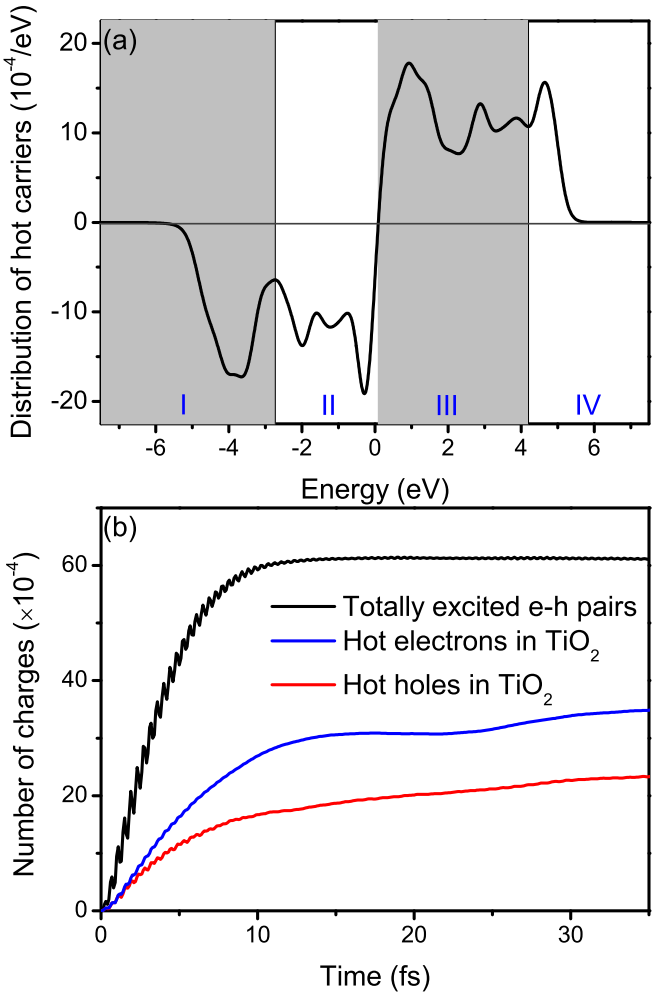

Figure S4: The hot carrier distribution at 30 fs (a) and the numbers of totally excited electron-hole pairs, hot holes and hot electrons in the TiO_2 (b) for the Al_{32}-TiO_2 system. The excitation frequency is 4.95 eV.

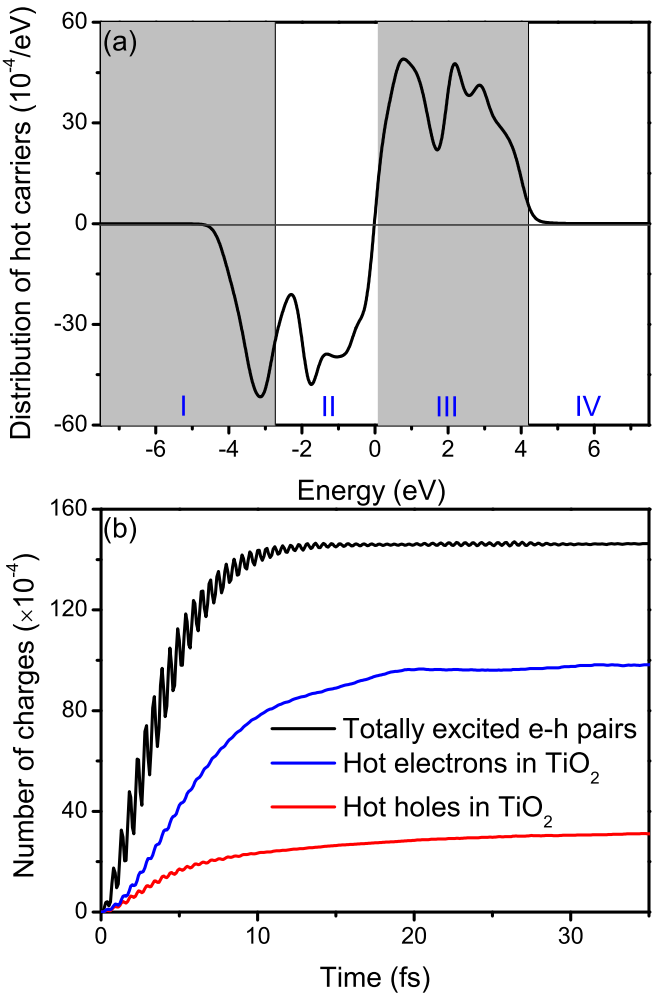

Figure S5: The hot carrier distribution at 30 fs (a) and the numbers of totally excited electron-hole pairs, hot holes and hot electrons in the TiO_2 (b) for the Al_{50}-TiO_2 system. The excitation frequency is 4 eV.

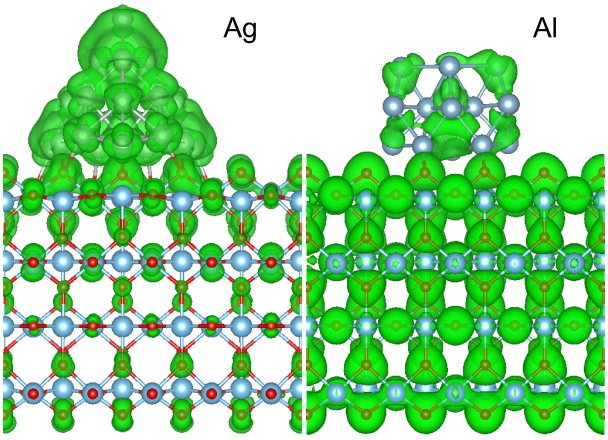

Figure S6: The charge densities of the region I hot carriers for the Ag-TiO_2 (left panel) and Al-TiO_2 (right panel) systems. The charge density is more localized on the Ag nanocluster than on the Al nanocluster, due to the *d*-band character in Ag.