Viable approach toward efficient *p*-type conductivity in Al-doped anatase TiO_2 via strain engineering

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The Al doping do not significantly modify the band edge electronic structures because of much lower content of Al *sp* states than that of Ti 3*d* states as shown in Fig. S1. Thus, we ignored their contributions to the band edge character in our discussions.

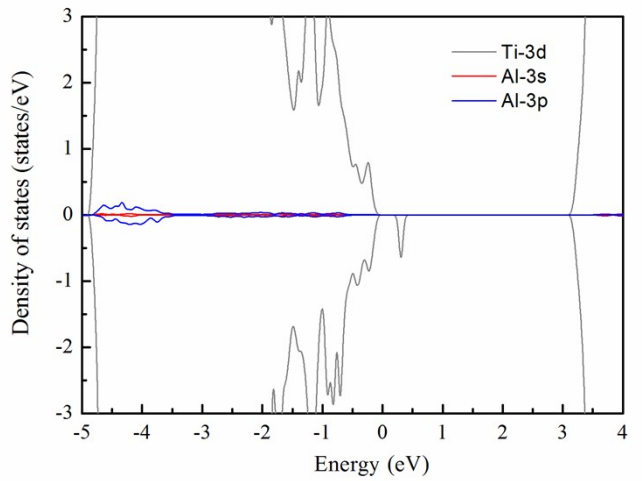

Fig. S1 Density of states for Ti-3*d*, Al -3*s* and -3*p* orbitals in Al doped TiO_2.

The density of states for Al-3*s*, 3*p* orbitals from LDA+U (U=0 for Al orbitals) and HSE06 calculations are shown in the Fig. S2 below. It can be seen that the top of valence band, which is our focus and plays key role in this work, are similar for both calculation results. Besides, the contribution of Al states is much smaller than that of Ti-3*d* states in the top of the valence band. Therefore, the standard LDA functional chosen for Al 3*s* and 3*p* electrons is reasonable and acceptable.

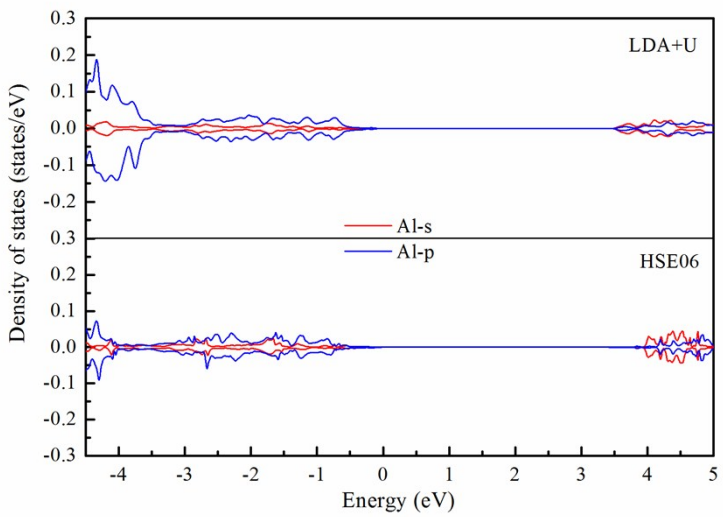

Fig. S2 Density of states for Al-3*s* and -3*p* orbitals in Al doped TiO_2 from LDA+U and HSE06 functional calculations, respectively.