Photocatalytic Properties of ZnO: Al/$MAPbI_3$/Fe_2O_3 Heterostructure: First-Principles Calculations

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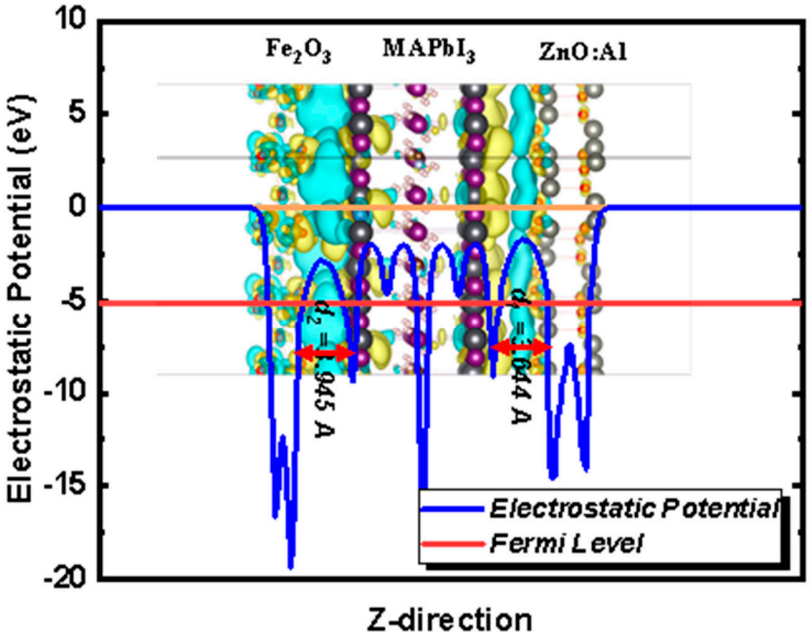

Figure S1: The work function of Fe_2O_3/$MAPbI_3$/ZnO:Al heterostructure. The red and yellow lines denote the Fermi level E_F, and the vacuum energy level E_{vac}, respectively and planar-averaged electron density difference in blue.

Equations used to compute different physical properties given in the manuscript

$$p_{S_2} = p_{D_2} \times e^{\frac{qV_{bi2}}{K_B T}}$$

$$p_{D_2} = N_{C2} \times e^{\frac{E_{F02} - E_{C02}}{K_B T}}$$

$$V_{bi_{12}} = E_{F02} - E_{F01}$$

$$n_{S_2} = n_{D_2} \times e^{\frac{-qV_{bi2}}{K_B T}}$$

$$n_{D_2} = N_{C2} \times e^{\frac{E_{F02} - E_{C02}}{K_B T}}$$

$$V_{bi_{12}} = E_{F02} - E_{F01}$$

Equations used to compute for H_2 production yield by rate of generation of excess carriers (unit volume/time):

$$\Delta i_{ph} = V \Delta G$$

$$\Delta G = \frac{A}{w} \Delta \sigma$$

$$\Delta \sigma = q(\mu_n + \mu_p) \Delta n$$

$$\Delta n = \tau_n \Delta G_L$$

Generation rote due to light:

$$\Delta G_L = \frac{\eta \Delta P}{h\nu A w}$$

$$\Delta i_{ph} = V \frac{A \tau_n}{W} q(\mu_n + \mu_p) \frac{\eta \Delta P}{h\nu A w}$$

$$\Delta i_{ph} = \frac{\Delta Q}{\Delta t} = \frac{\eta \Delta P \, q}{h\nu} \left(\frac{\tau_n}{t}\right)$$

$$n_e = \frac{\Delta Q}{q} = \frac{\eta \Delta P}{h\nu} \left(\frac{\tau_n}{t}\right) \Delta t$$

$$\Delta n = \Delta p$$

$$n_0 = N_C e^{\frac{-(E_C - E_F)}{K_B T}}$$

$$\Delta n = n_0 e^{\frac{-qV_{bi}}{K_B T}}$$

$$N_C = 2\left(\frac{2\pi m_e^* K_B T}{h^2}\right)^{\frac{3}{2}}$$

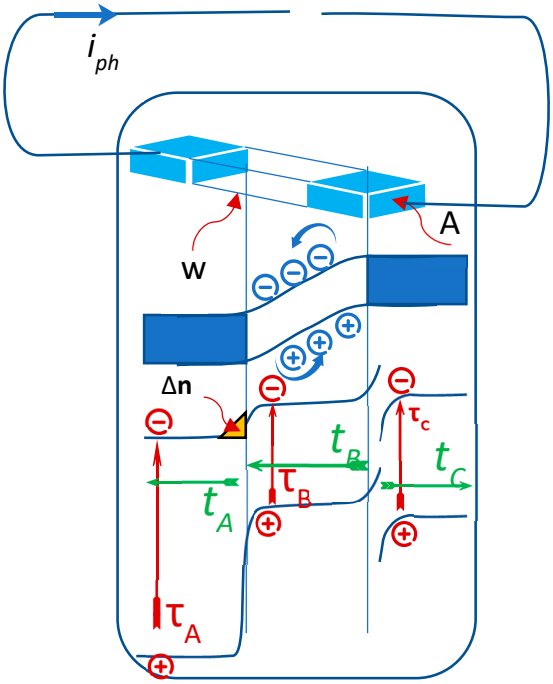

Figure S2: Fe_2O_3/$MAPbI_3$/ZnO:Al heterostructure schematic and photocatalytic activity measurements set up