Title: **Effects of p-type (Ag, Cu) dopant on the electronic, optical and photocatalytic properties of MoS_2, and impact on Au/$Mo_{100-x-y}Ag_xCu_yS_2$ performance(Article)**

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Abstract

MoS_2 is an alternative of graphene due to its intriguing properties and it is necessary to modify the properties for achieving p-MoS_2 and complementary device applications. Doping is one of the most prevalent techniques for modification of materials properties and fabricating p-MoS_2. Herein, we report on Ag and Ag-Cu doped MoS_2 investigated by theoretical and experimental studies. Detailed study of DFT highlights the confirmation of p-type MoS_2. The band gap can be tuned from 1.21 to 0.51 eV (theoretically) and 1.92–1.30 eV (experimentally). The enhancement of absorption in the visible region attributed to Ag and Ag-Cu doping. The conduction band (CB) edge potential is smaller in negative than H^+/H_2 (0.0 eV) for undoped, Ag = 2.5% and Ag-Cu (Ag = 2.5, Cu = 10%) doped MoS_2, hence the photogenerated electrons can weakly reduce H^+ to produce H_2. While the deeper valence band (VB) edge potential than O_2/H_2O (1.23 eV) confirms that the holes created upon photon absorption strongly shows the ability for water oxidation. However for other doping both potential edges are more positive which insights strong oxidative material. Interestingly, the theoretical calculation suggests that the CB edge potential should be upward shifting for enhancing the photocatalytic activity of MoS_2. EDX and XPS measurements disclose the presence of Mo, S, Ag and Cu elements in the thin films. Furthermore, decreasing forward current and shifting threshold voltage (V_T) toward higher voltage in (Ag, Cu) doped Au/$Mo_{100-x-y}Ag_xCu_yS_2$ insights p-type MoS_2. Therefore, these demonstrations could be extended its applications to be enable high-performance electronic and optoelectronic devices. © 2020

Author keywords

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