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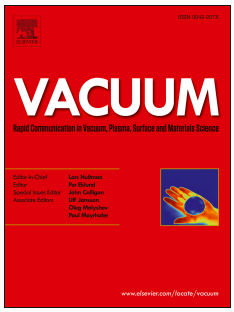


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# Optical absorption enhancement of Hg-doped ZnX (X= S, Se) for hydrogen production from water splitting driven by solar energy

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## ABSTRACT

ZnX (X= S, Se) can perform photocatalytic hydrogen generation from water splitting. However, the reaction cannot be driven by solar energy because of the wide band gaps of ZnX. To tune their photocatalytic activity for the hydrogen generation driven by solar energy, we investigate the geometrical structures, the electronic, optical and photocatalytic properties of Hg-doped ZnX by using the first-principles density functional theory calculation with the meta-GGA+MBJ potential. Four concentrations of Hg dopants are considered. The carrier mobility and the recombination of the hole and electron are calculated and used to evaluate the photocatalytic activity of the structures. The results demonstrate that the formation energies of the doped structures are small, which implies that the synthesis of these materials is not difficult in energy. The energy band gaps of ZnX decrease along with the increase of the doping concentration, and the smallest one still satisfies the requirement of photocatalytic water splitting. Additionally, the optical absorption of the Hg-doped ZnSe in the near ultraviolet and visible light range increases significantly. The obvious charge difference and the relative ratio of electron and hole are observed. Therefore, Hg-doped ZnSe is a potential candidate for hydrogen

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