Colloidal-quantum-dot gas sensors using atomic-ligand engineering

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Colloidal quantum dots (CQDs) have attracted considerable attention owing to their large surface area and abundant dangling bonds[1]. The surface ligand of CQDs play a vital role in their chemical activity, electronic structure, and gas sensing performance[2]. In this paper, lead sulfide (PbS) colloidal quantum dots were selected as the research object, and the oleic acid ligand was removed from the CQD surface of lead sulfide (PbS) by the phase-transfer ligand exchange strategy. Meanwhile, halogen ligand (Cl, Br, I) was introduced to passive the quantum dot surface, taking into account the surface activity and chemical stability. Real-time electrical measurement combined with in situ diffuse reflection Fourier transform infrared spectroscopy analysis showed that the films prepared by the PbS colloidal quantum dots exhibited p-type conductivity in air and had a significant response to NO_2 gas at room temperature, as while as the long-term stability of the sensor was improved. Density functional theory calculations show that halogen ligands have good surface passivation effect on PbS quantum dots. The microscopic mechanism of gas sensitivity of different halogen ligands to PbS colloid quantum dots is further compared and analyzed. The results show that the surface ligand engineering of CQDs is helpful to the design and fabrication of gas sensors with high sensitivity and reliability and can be used to improve the stability of various colloidal quantum dot devices.

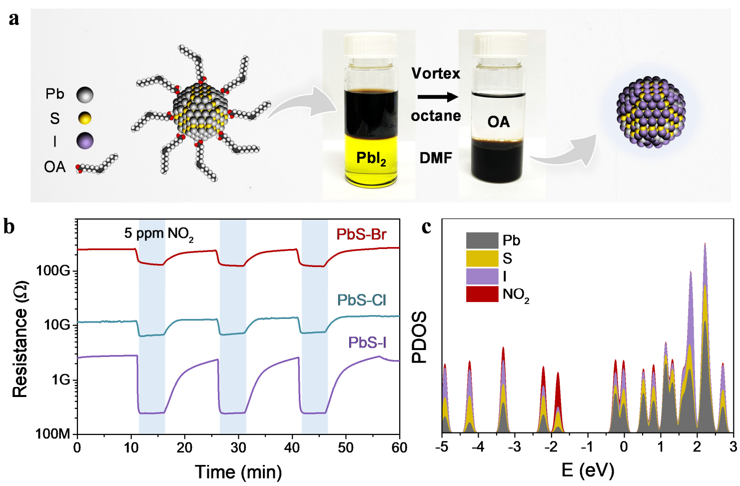

Fig. 1. (a) Phase transfer ligand exchange strategy to remove oleic acid ligand from PbS CQD surface and introduce halide ligand to passivate the surface, (b) Response of PbS CQD gas sensors treated with different halogen ligands (Cl, Br, I) to 5 ppm NO_2 at room temperature, (c) The project density of state (PDOS) of PbS colloidal quantum dots treated with I ligand.

[1] Liu H, Li M, Voznyy O, et al. Physically flexible, rapid-response gas sensor based on colloidal quantum dot solids. Adv Mater, 2014, 26: 2718–2724.

[2] Russ T, Hu Z, Junker B, et al. Operando investigation of the aging mechanism of lead sulfide colloidal quantum dots in an oxidizing background. J. Phys. Chem. C, 2021. DOI: 10.1021/acs.jpcc.1c04045