Surface and grain boundary defect passivation in perovskite solar cells using infrared-absorbing aza-dipyrromethene fluorophore

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Introduction

Since 2009, perovskite solar cells (PSCs) have witnessed dramatic developments with the record power conversion efficiency (PCE) exceeding 25% in the past ten years.[1-3] One bottleneck for the commercialization of PSCs is the instability caused by hole transport materials (HTMs) with dopants .[4] These dopants are usually hygroscopic and deteriorate the long-term stability by moisture ingress and ion diffusion. In addition, The dopants also increase the device complexity and total cost of PSC_S. [5] accordingly, the development of dopant-free HTMs is of great significance. In this work, we report a series of new HTMs with a molecular design concept to enhance their light absorption in the near infrared region (NIR) and their ability of passivation of surface defects of perovskite layer by metal–ligand interaction. The perovskite solar cells based on the HTMs of aza-dipyrromethenes **1-3** achieved the championship PCE of 18.6%, 17.3%, and 19.4%, respectively.

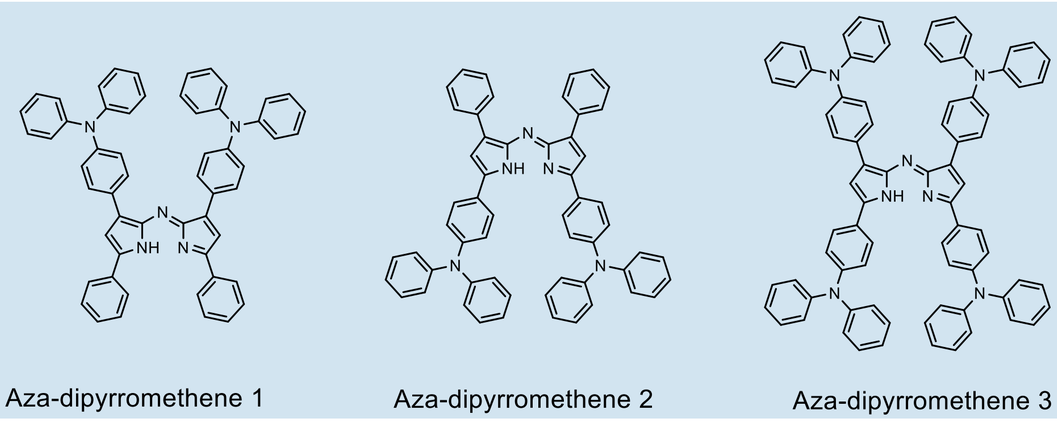
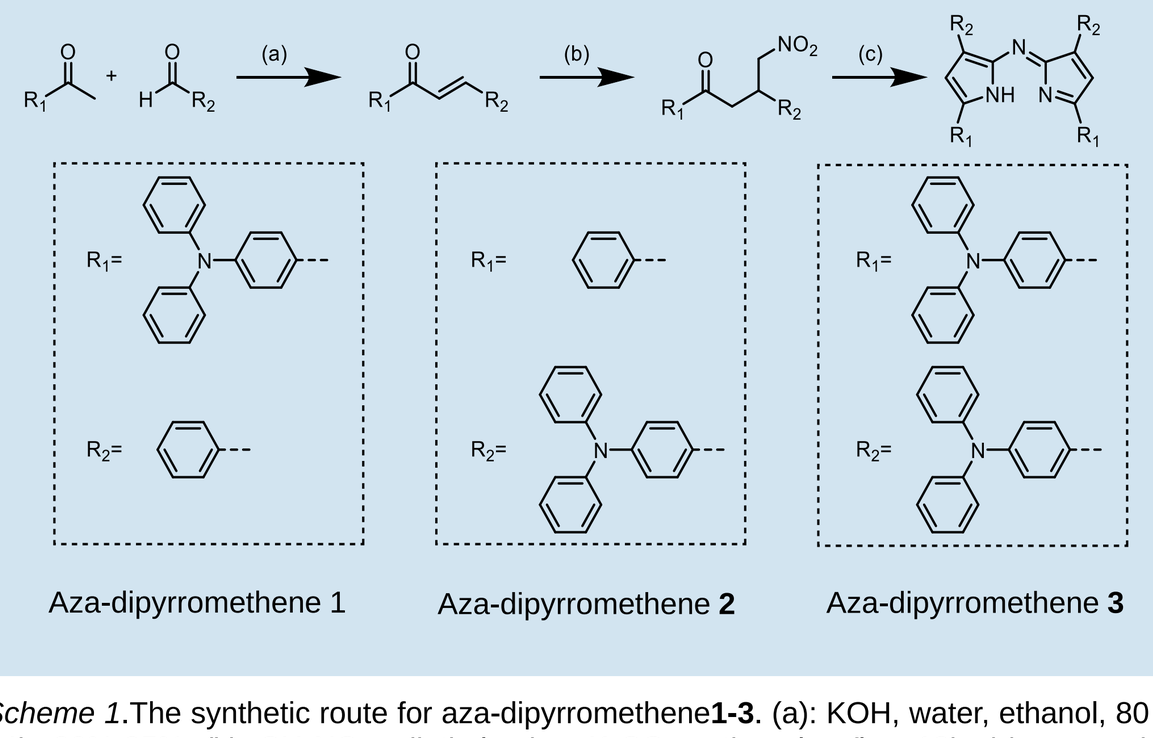


Fig. 1: Chemical structures of aza-dipyrromethene **1-3**.

Results and discussion



Scheme 1.The synthetic route for aza-dipyrromethene**1-3**. (a): KOH, water, ethanol, 80 ℃, 24h, 90%-95%; (b): CH_3NO_2 , diethylamine, K_2CO_3 , ethanol, reflux, 12h; (c): ammonium acetate, *n*-butanol, 110℃, 12 h, 80%–90%.

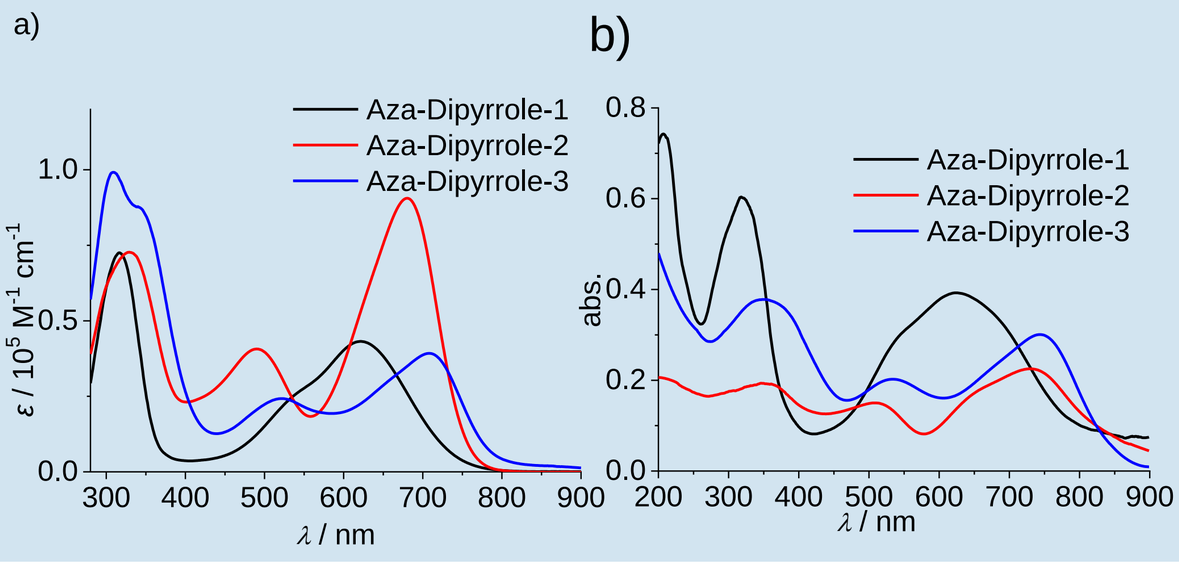


Fig. 2: a) UV/Vis absorption spectra of aza-dipyrromethene **1-3** in CH_2Cl_2(1.0 ×10^{-5} M). b) UV/Vis absorption spectra of thin film of dipyrromethene **1-3**.

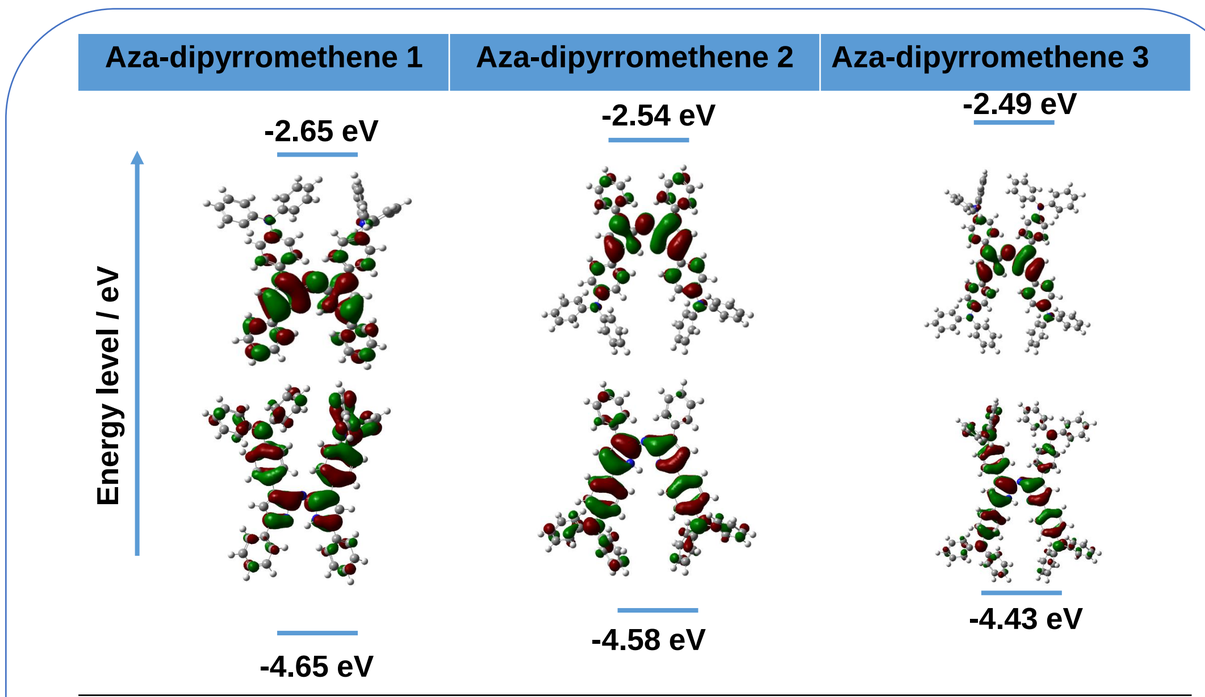


Fig. 3: The calculated HOMOs and LUMOs of compounds aza-dipyrromethene **1-3**.

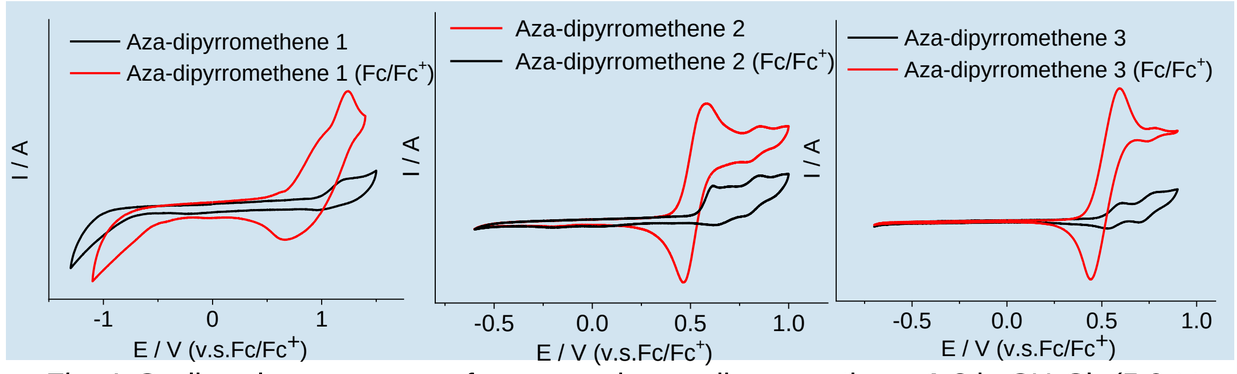


Fig. 4: Cyclic voltammograms of compounds aza-dipyrromethene **1-3** in CH_2Cl_2 (5.0 × 10^{-4} M). The scan rate is 50 mV/s. Ferrocene was used as internal reference.

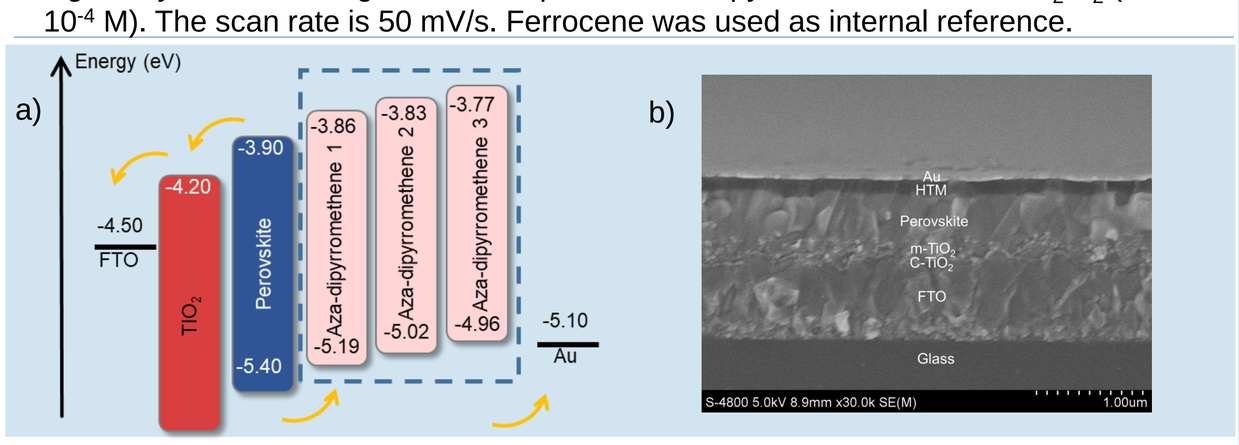


Fig. 5: a) Energy levels diagram of PSCs based on different HTMs. b) Device structure.

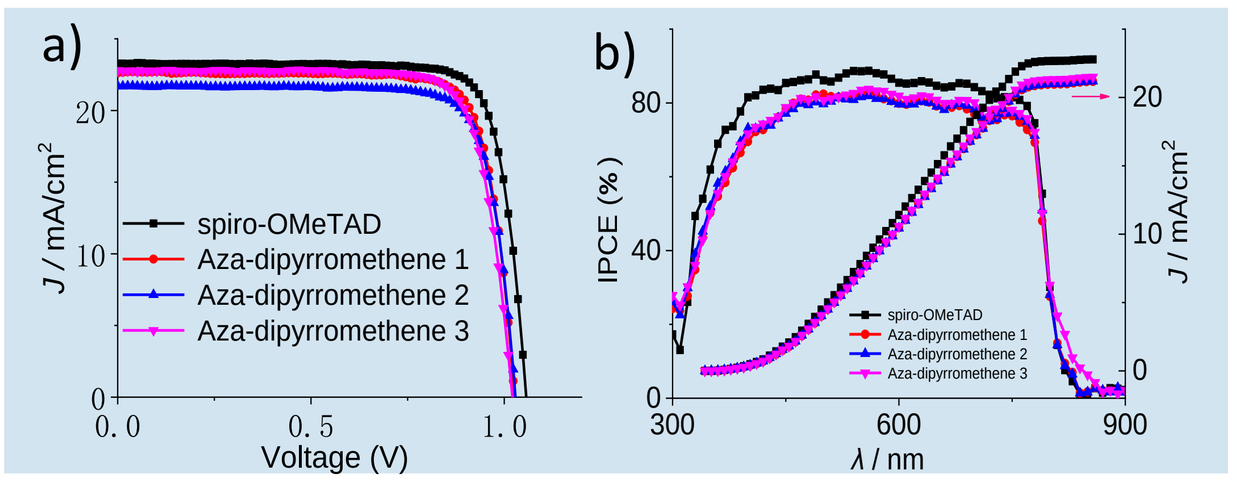


Fig. 6: a)*J*−*V* curves of the champion PSC based on dopant additive-free aza-dipyrromethenes and spiro-OMeTAD HTM. b) IPCE curve and J_{sc} integration of the champion PSC.

Conclusion and Outlook

In summary, we have designed and synthesized three undoped HTMs for perovskite solar cells. A series of aza-dipyrromethenes bearing triphenylamine moities synthesized and characterized. These HTMs as well as exhibit NIR absorption properties and suitable energy levels. The efficiency of these three HTMs comparable to doped spiro-OMeTAD was obtained. The long-term stability of the PSCs based on the new HTMs are under investigation.

References

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