Dual-Site Passivation of Tin-Related Defects Enabling Efficient Lead-free Tin Perovskite Solar Cells

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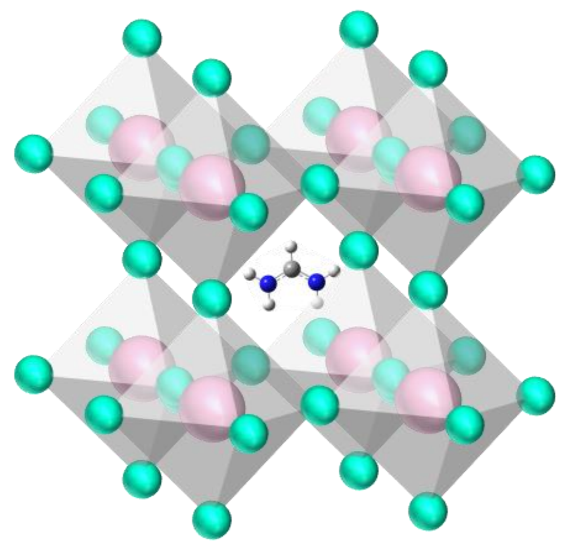
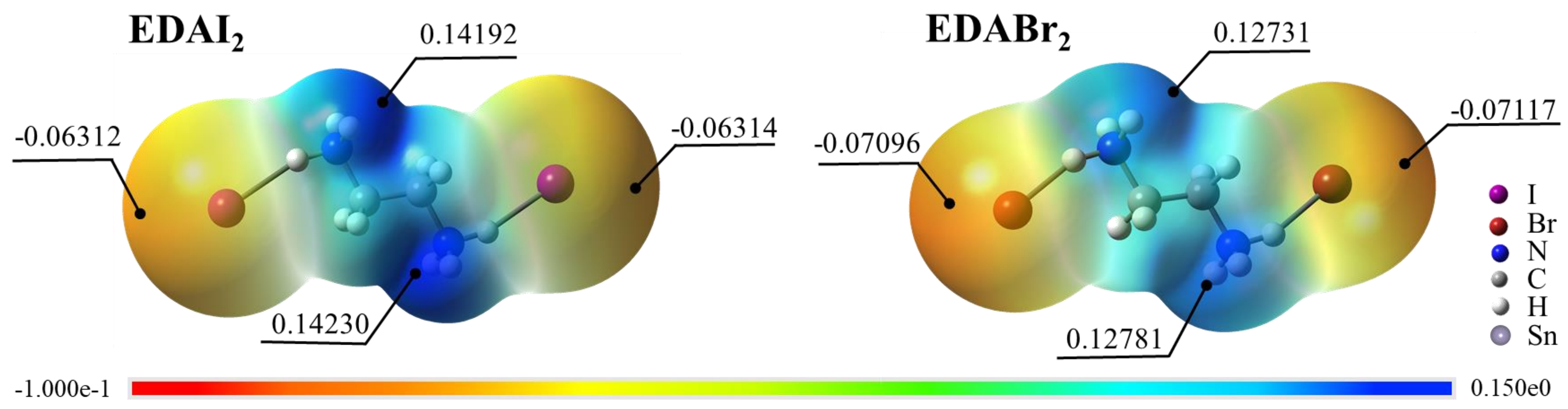
Challenging issues



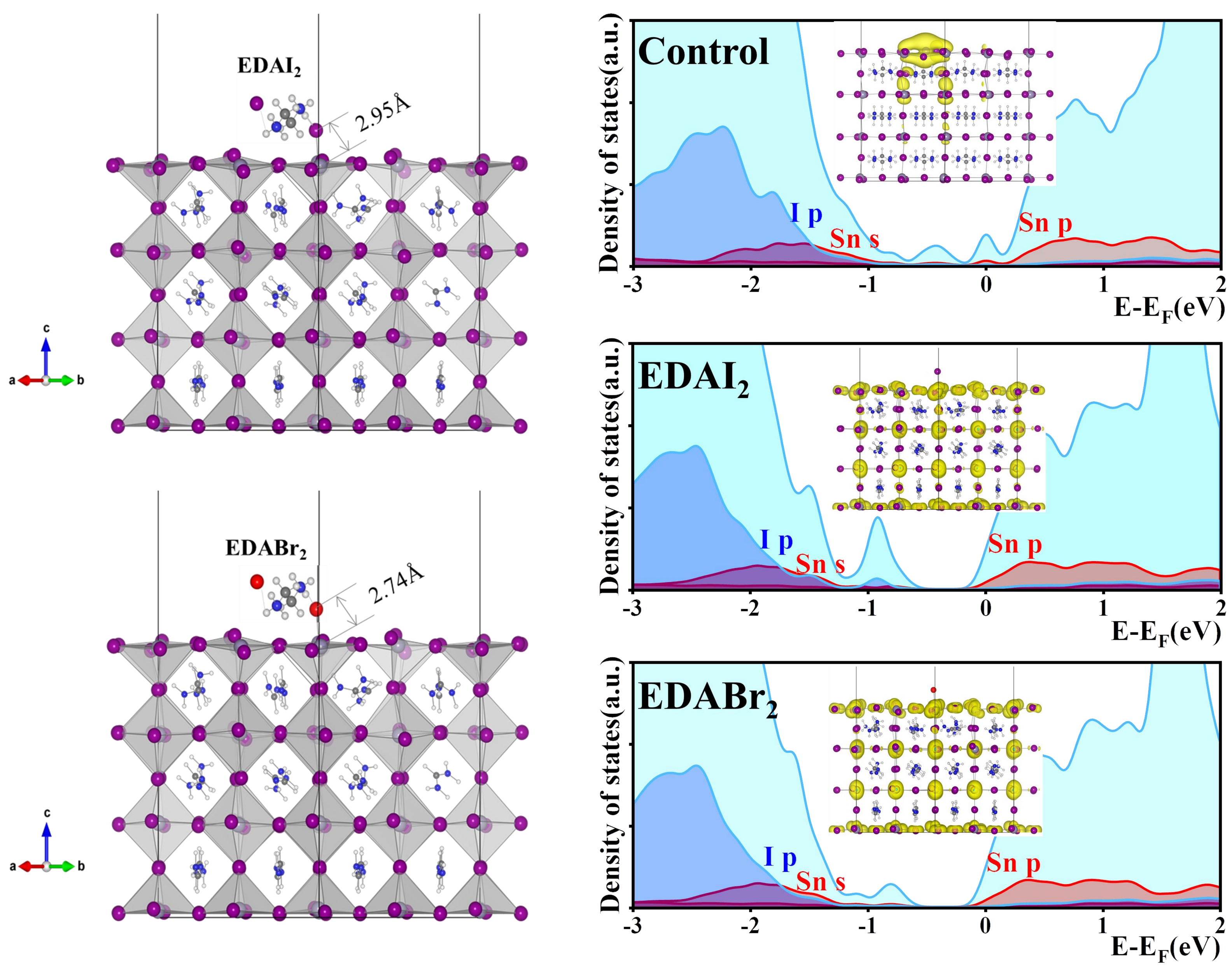
- Easy oxidation of Sn^{2+} to Sn^{4+}, especially at the surface;
- Intrinsic point defects, such as antisite substitutions (e.g., Sn_I antisite) and undercoordinated Sn^{2+} (e.g., Sn_i interstitial);
- Grain boundaries (GBs) caused by the small grains during fast crystallization;
- These deep-level defects act as primary non-radiative recombination centers, impairing the efficiency and stability of Sn-based perovskite solar cells.

Results and discussion

Sn_I antisite defects passivation

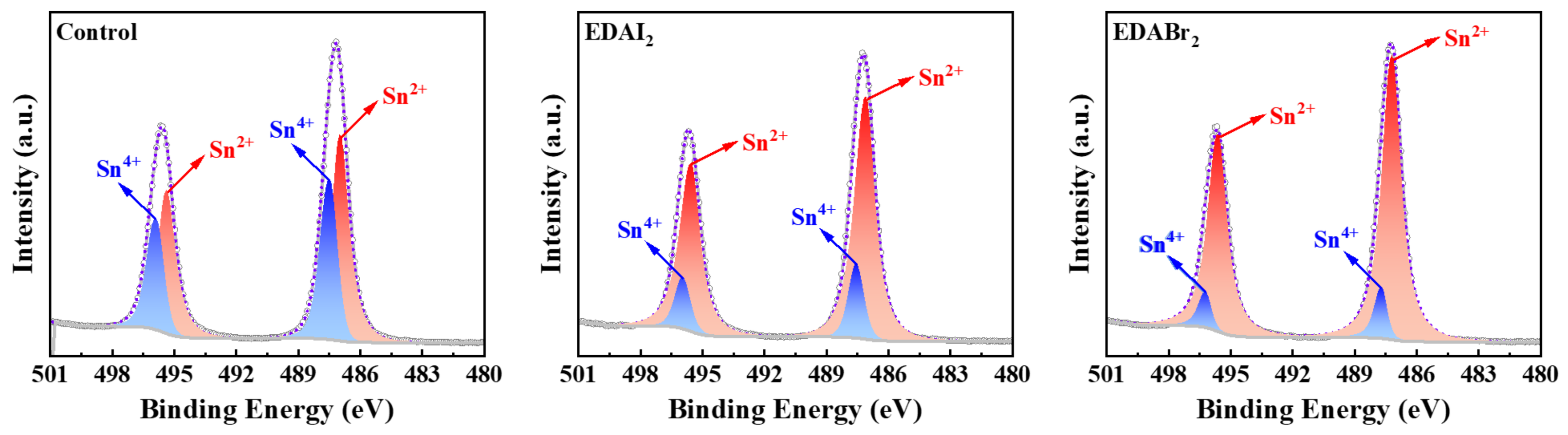


- Larger absolute electrostatic potential determined stronger electron-withdrawing property at the halide terminals.

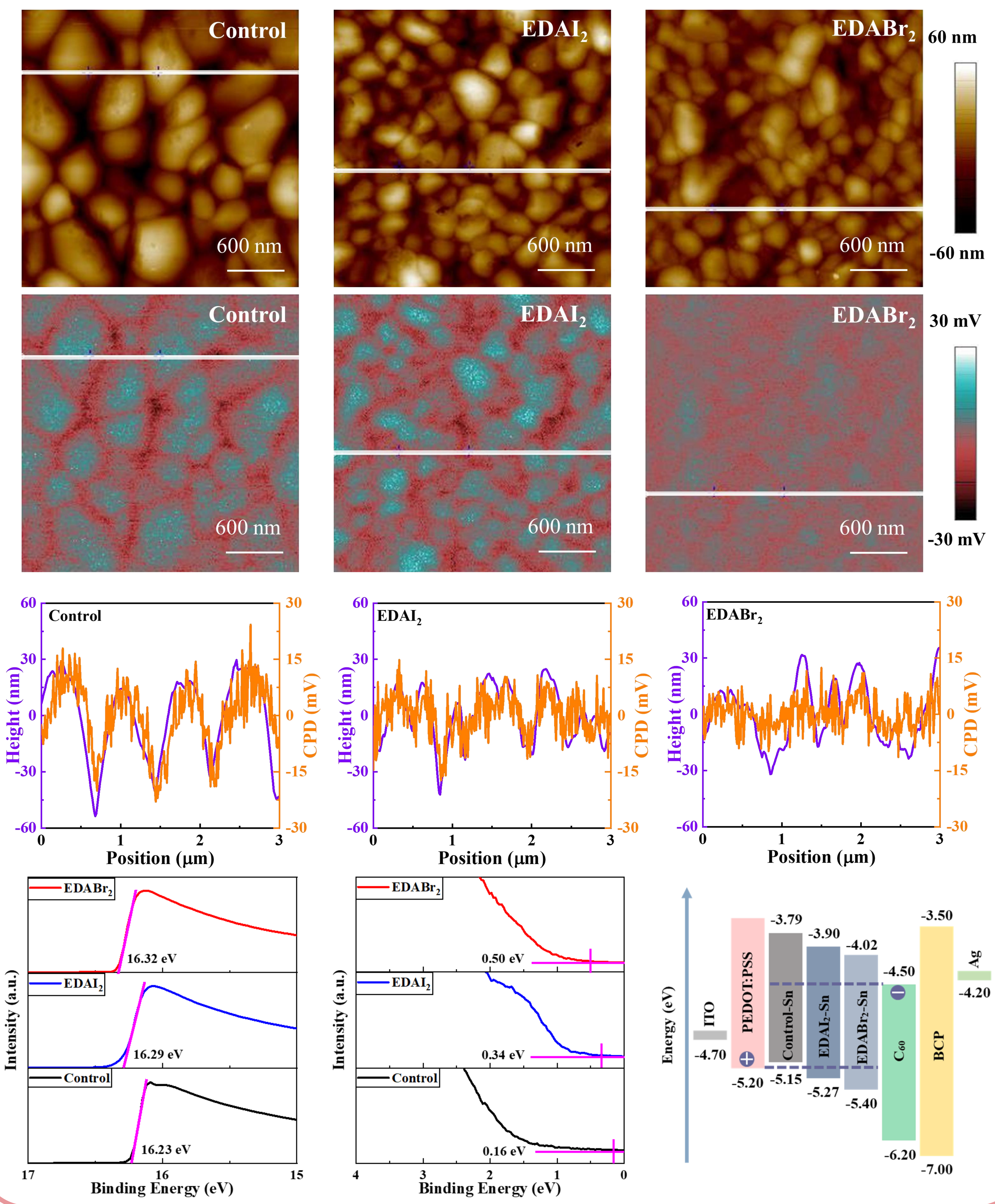


- Better molecular adsorption between $EDABr_2$ and $FASnI_3$ (001) surface structures;
- EDA-based molecules could passivate Sn_I antisite defects, and $EDABr_2$ molecule eliminate more trap states in the gap close to the VBM.

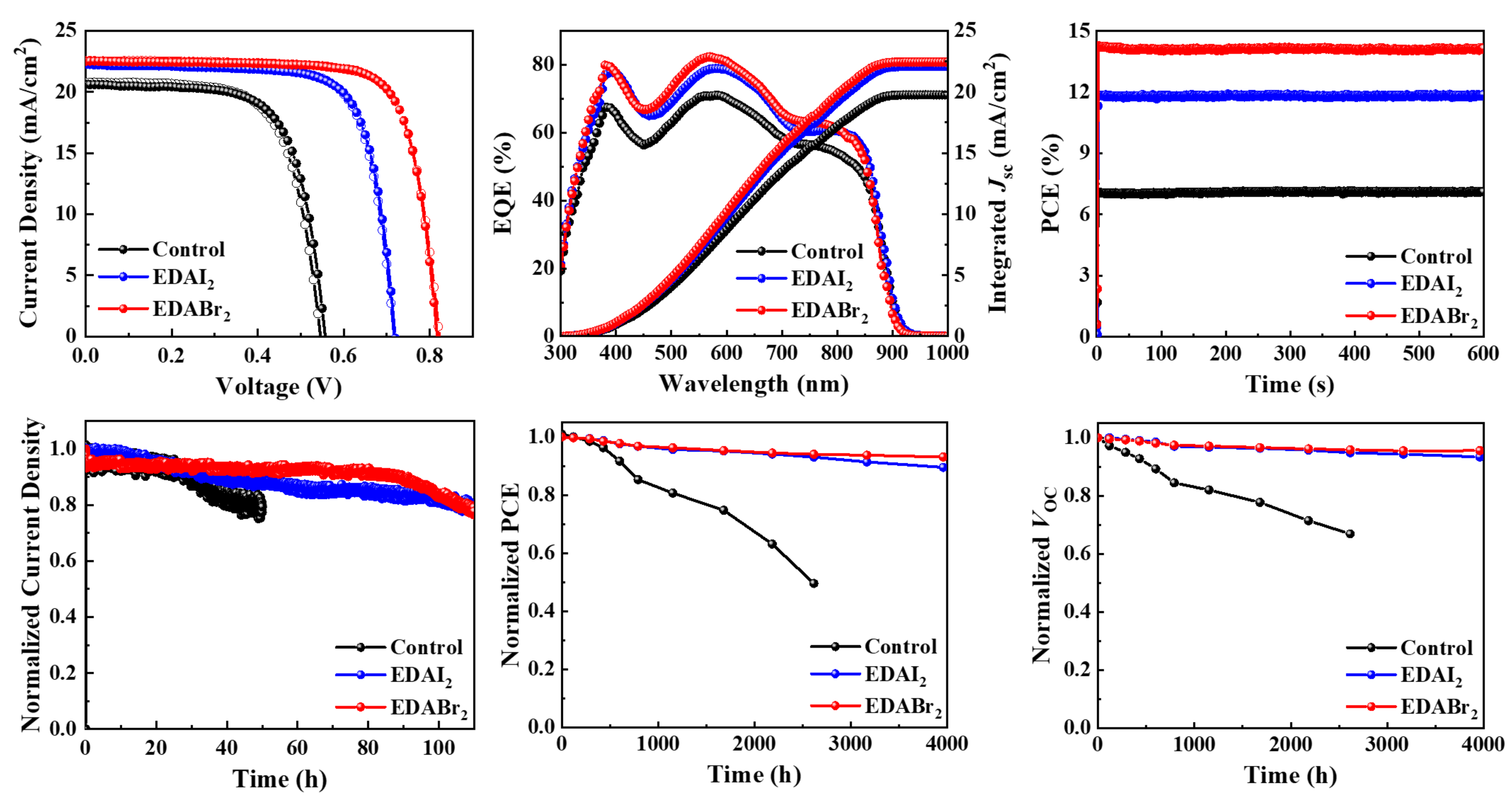
Oxidation prevention



Grain boundary passivation



Device perfromance



Conclusion and acknowledgments

- $EDABr_2$ effectively prevents Sn^{2+} oxidation, leading to reduction of Sn vacancies both at surface and bulk perovskite.
- $EDABr_2$ exhibits more consummate passivation effect than $EDAI_2$ on Sn_I antisite defects as deep-level traps.
- The champion $EDABr_2$-modified perovskite solar cells achieves a greatly enhanced PCE of 14.23% with excellent stability.
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