Innov Ener Res 2018, Volume 7
DOI: 10.4172/2576-1463-C1-003

Advanced Energy Materials and Research

Elucidating the role of Sn-substitution and Pb-Vc in regulating stability and carrier concentration in CH3NH3Pb1īXīYSnXVcYI3

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Inorganic-organic perovskites, $CH_3NH_3PbI_3$ in particular, have recently drawn signi cant attention in improving solar cell's performance due to their long di usion length, high carrier mobility, suitable optical band gaps, and strong absorption of light. However, the presence of Pb has rendered its usage in developing non-toxic lead-free devices. erefore, reducing the extent of Pb by substituting a suitable alternative metal (e.g. Sn, Ge, Sr, etc.) in the perovskite has become extremely important. Moreover, inclusion of Sn in the perovskite network (i.e. $CH_3NH_3Pb1{-}xSn_xI_3$) can reduce the optical band gap. is enables the perovskite to absorb all visible lights of the solar spectrum along with some ultraviolet to near-infrared photons (up to 1.1 eV). erefore, digging deep into the atomistic insights and electronic structure of Sn based perovskites has become profoundly important for designing e cient energy harvesting materials. In this talk, I shall address the role of Sn-substitution and Pb-vacancy (Vc) in regulating stability and carrier concentration of $CH_3NH_3Pb1{-}X{-}YSn_XV_{cY}I_3$ using state-of-