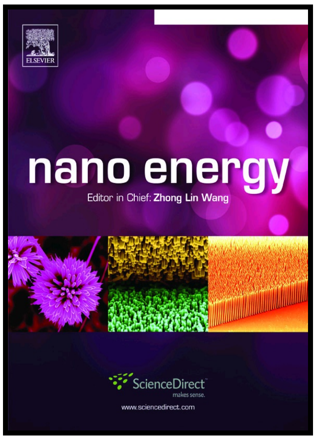

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Modulations of various alkali metal cations on organometal halide perovskites and their influence on photovoltaic performance

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Keywords: Alkali metal cations, perovskite solar cells, defect, hysteresis, high efficiency

Abstract: The crystal structure and properties of organometal halide perovskites incorporating various alkali metal cations were systematically investigated. The X-ray diffraction results suggested that the lattice constant of the perovskites incorporating Li^+, Na^+ or K^+ is larger than that of the perovskite without incorporation, while the incorporation of Rb^+ or Cs^+ did not change the lattice constant. The incorporation of Li^+, Na^+ or K^+ resulted in a red shift in absorption edge, whereas the incorporation of Rb^+ or Cs^+ caused a blue shift. The identical trend was also found in the photoluminescence spectra, indicating the modification of the band gap by the alkali cations. The valence band maximum and conduction band minimum of the perovskites containing Li^+, Na^+ or K^+ were upshifted, while those were downshifted in the Cs^+ case. The assessments of the carrier lifetime and the defect revealed that the K^+ containing perovskite had the least defect, followed by the perovskites containing Rb^+, Cs^+ and Na^+. In addition to the barrier at the perovskite/TiO_2 interface, the defects in perovskites played a crucial role in hysteresis in the current versus voltage curves. Consequently, the efficiency of more than 20% with negligible hysteresis was achieved in K^+ containing perovskite solar cells.