

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Ion Migration in Lead-Halide Perovskites: Insights from First-Principles Calculations DAVID A. EGGER, Weizmann Institute of Science, SUBHAM DASTIDAR, Drexel University, LIANG Z. TAN, University of Pennsylvania, SAMUEL B. CROMER, ANDREW D. DILLON, Drexel University, SHI LIU, Carnegie Institution for Science, AARON T. FAFARMAN, Drexel University, ANDREW M. RAPPE, University of Pennsylvania, LEEOR KRONIK, Weizmann Institute of Science — Lead-halide perovskites (LHPs) are promising semiconductors especially for efficient solar cells. However, LHP cells show hysteresis in the current-voltage curves and their stability with respect to water exposure is problematic. These issues are possibly related to defect migration occurring in the perovskite material [1]. Here, we present our first-principles results on defect migration phenomena in hybrid and all-inorganic LHPs.[2,3] Our calculations are based on density functional theory and nudged-elastic band methods to optimize minimum energy pathways of defect species. First, the migration of hydrogen interstitials is discussed,[1] where we find that migration barriers are small, indicating mobile hydrogen interstitials at room temperature. Second, results on migration and anion-exchange reactions of interstitial Cl in all-inorganic CsPbI₃ are presented.[2] Cl migration is found to facilitate Cl doping at levels near the solubility limit for chloride in CsPbI₃. At these incorporation levels the stability of a CsPbI₃ film is strongly improved compared to an undoped film. References: [1] Egger et al., *Acc. Chem. Res.* 49, 573 (2016), and references therein. [2] Egger et al., *Angew. Chem. Int. Ed.* 54, 12437 (2015). [3] Dastidar et al., *Nano Lett.* 16, 3563 (2016).

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Date submitted: 10 Nov 2016

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