Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information:

Point defect mediated hot carrier relaxation dynamics of lead free $FASnI_3$ perovskites

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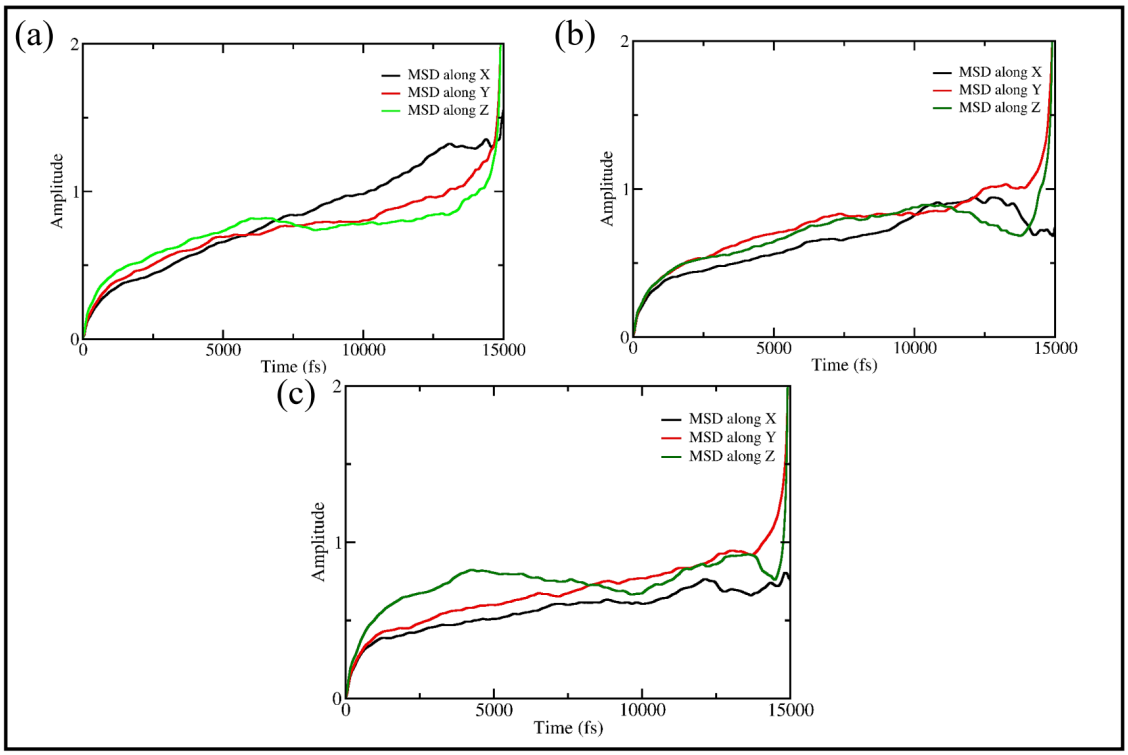

Figure S1: Mean square displacements of atoms during AIMD simulations (canonical ensemble) of (a) pristine, (b) Sn vacancy and (c) I vacancy $FASnI_3$ perovskites.

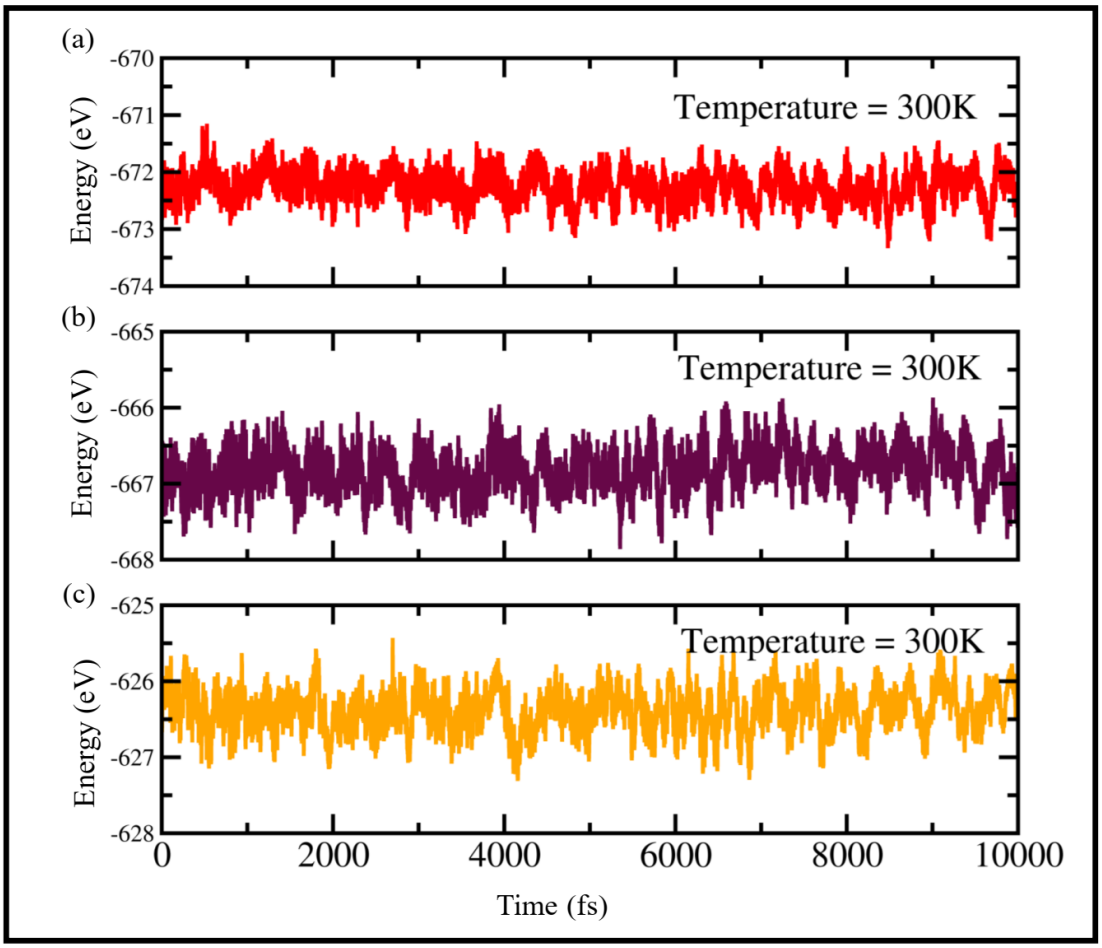

Figure S2: Potential energy evolution of (a) pristine, (b) Sn vacancy and (c) I vacancy $FASnI_3$ perovskite in microcanonical (NVE) ensemble.

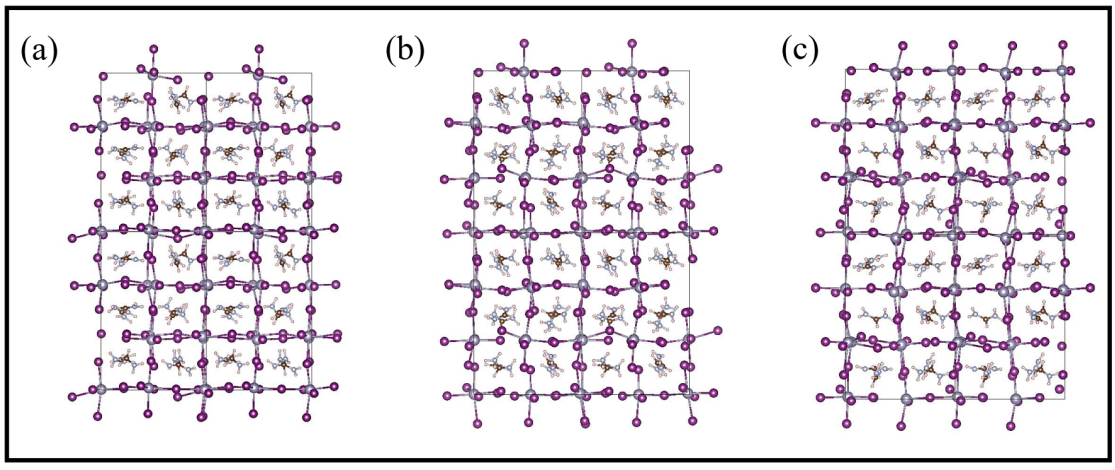

Figure S3: Time evoluted geometries of (a) pristine, (b) Sn vacancy and (c) I vacancy $FASnI_3$ perovskite after AIMD simulation in microcanonical ensemble.

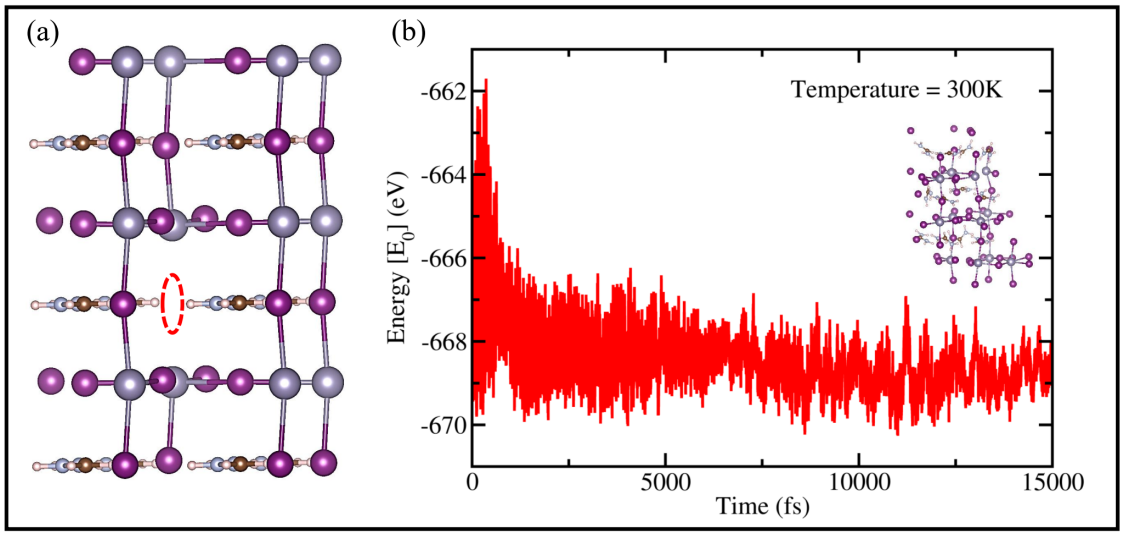

Figure S4: (a) Optimized structures of iodine vacancy $FASnI_3$ perovskite. The red dotted area represent the iodine vacancy. (b) Potential energy evolution of iodine vacancy $FASnI_3$ perovskite in canonical ensemble. The time evoluted geometry are attached inset.

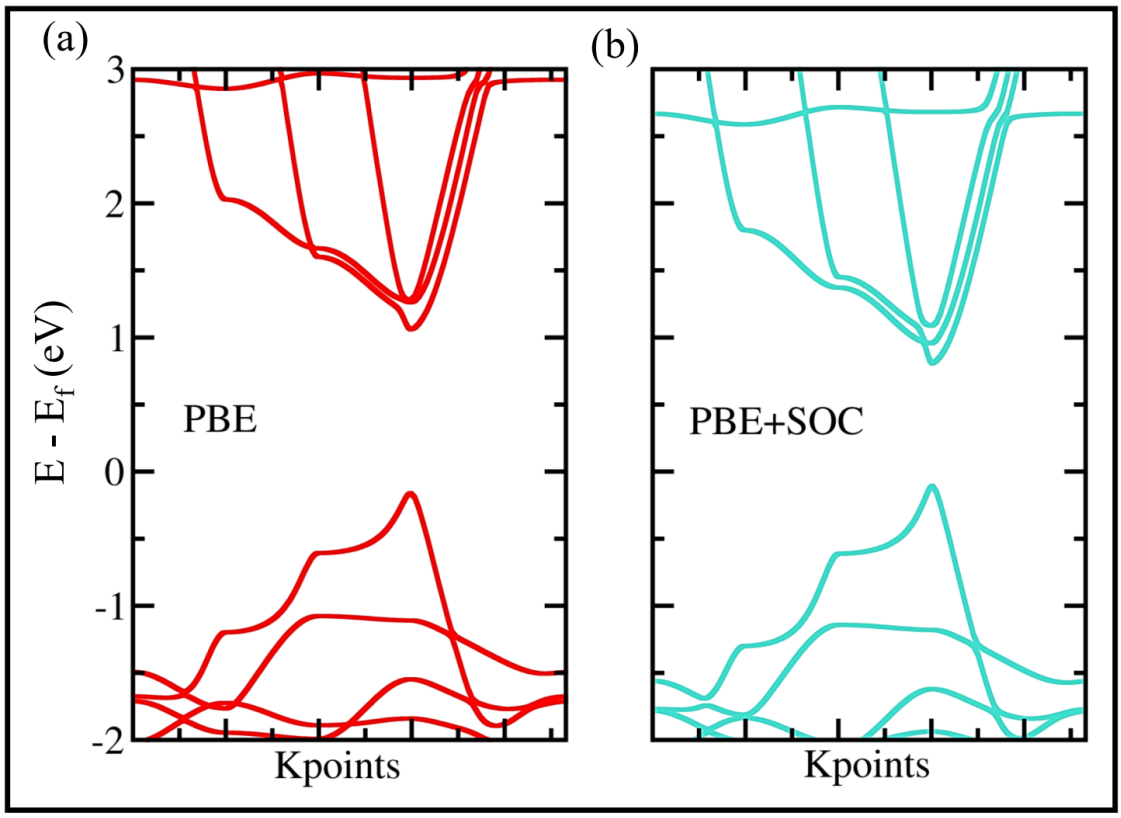

Figure S5: Band structures of the unitcell of pristine $FASnI_3$ using (a) PBE and (b) PBE + SOC (spin orbit coupling). Fermi levels are set to zero.

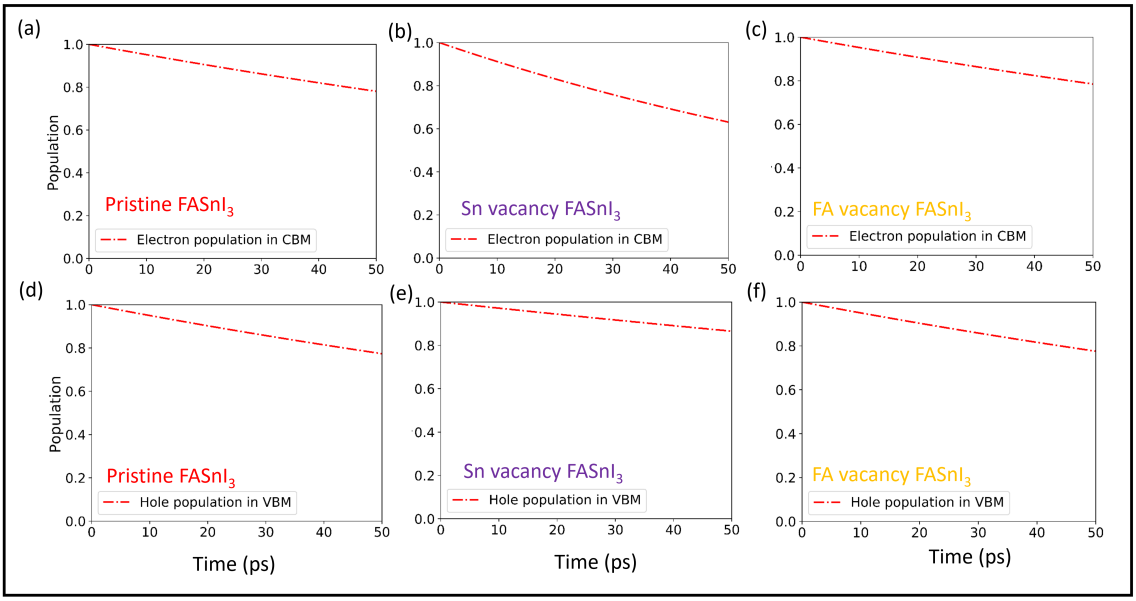

Figure S6: Population of hot electrons in upper CBM levels during NAMD simulation of (a) pristine (b) Sn vacancy and (c) FA vacancy $FaSnI_3$ perovskites. Population of hot holes in lower VBM levels during NAMD simulation of (a) pristine (b) Sn vacancy and (c) FA vacancy $FaSnI_3$ perovskites.