Supporting Information

Hysteresis and instability predicted in moisture degradation of perovskite solar cells

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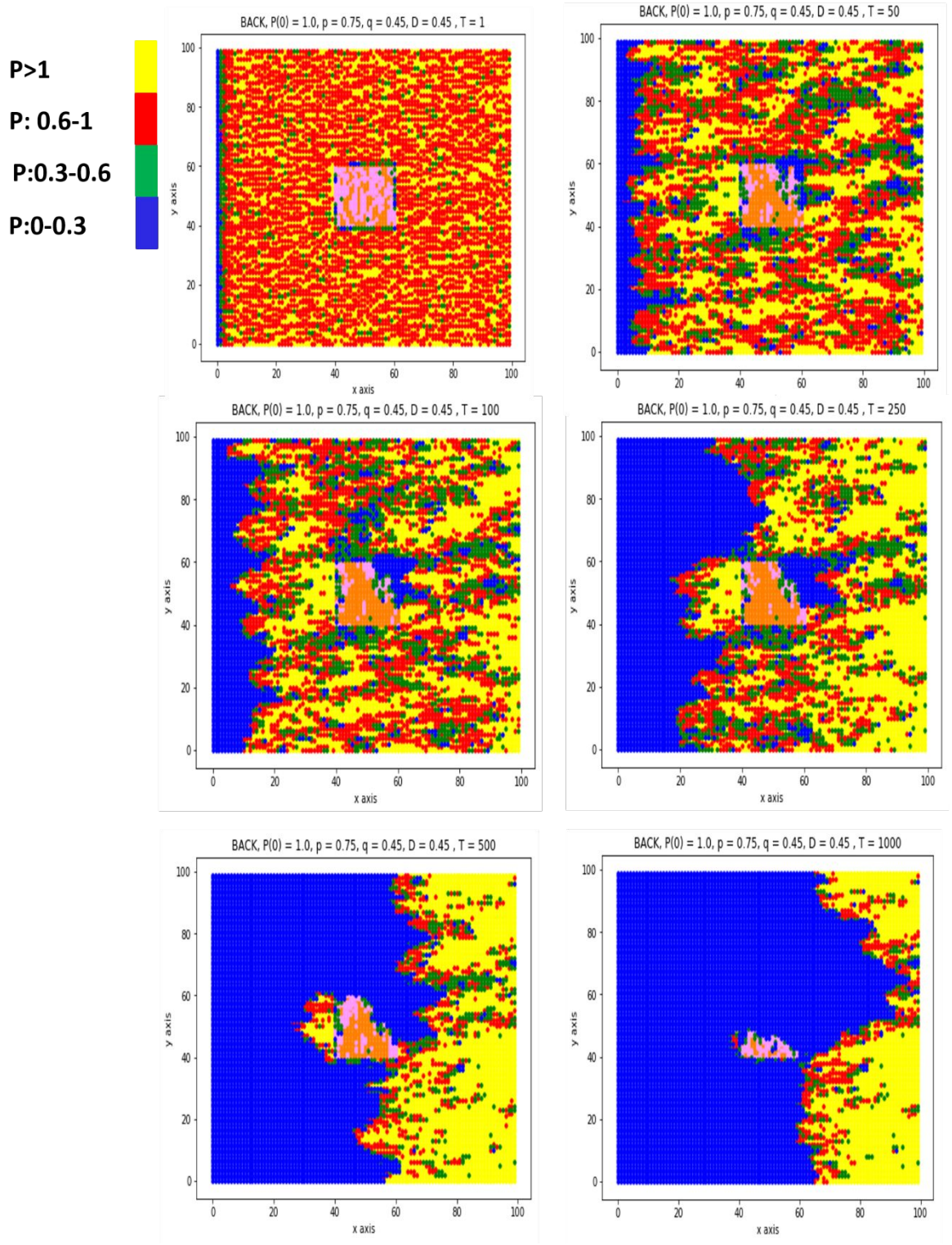

Figure S1. Time-resolved image for Figure 3c: the possibility of water back diffusion has been simulated, when the left boundary of the lattice was set to zero, after the complete saturation of all the Ps (=1.0). Only the P value were updated throughout the time iteration to simulate the back diffusion. These diagrams showed the time-resolved water diffusion process. Eventually, it was discovered that the diffusion seems to be localized within some area, or even become trapped in the area far away from the draining boundary.

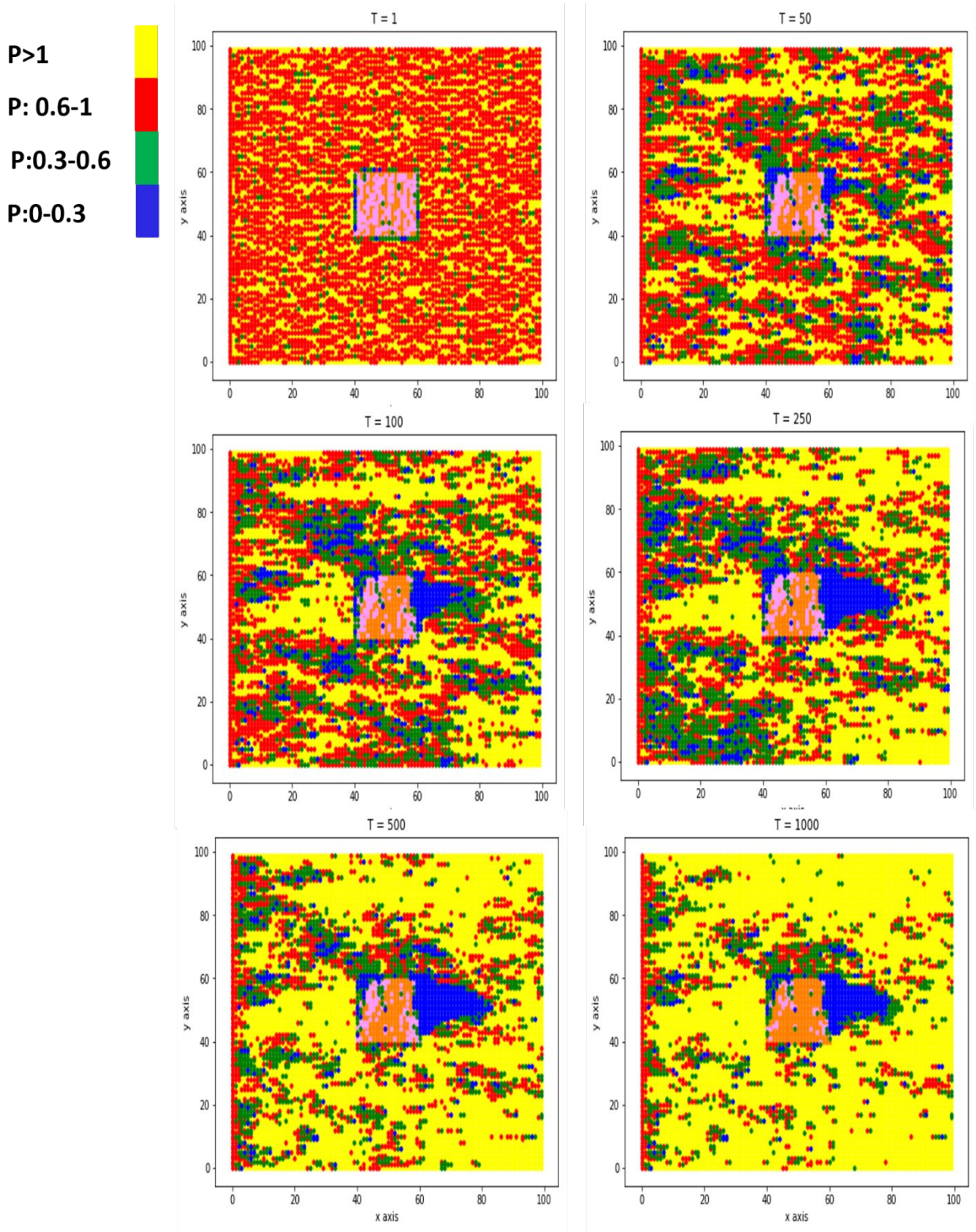

Figure S2. Time-resolved image for Figure 4b: All the P values were initialized to 1, including the boundaries. All the W values were then assigned by either 0 or 1, to mimic the potential instabilities under the presence of 1D PbI_2 chains. These diagrams showed the time-resolved water diffusion process, which seemed to be frozen, should such imbalance be regulated towards a certain orientation.