Supporting Information for

Understanding the Liquefaction in Halide Perovskites upon Methylamine Gas Exposure

Wencai Zhou^a, Zilong Zheng^{*a}, Yue Lu^{*a}, Manling Sui^a, Jun Yin^b and Hui Yan^a

^a Faculty of Materials and Manufacturing, Beijing University of Technology, Beijing 100124, China
^b Division of Physical Science and Engineering, King Abdullah University of Science and Technology, Thuwal 23955-6900, Kingdom of Saudi Arabia

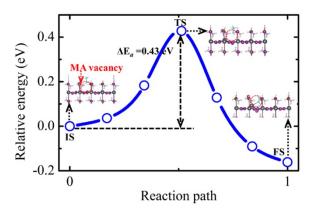


Fig. S1 Potential energy surface of methylamine gas molecule diffusion process, on the MA-vacancy perovskite surface.

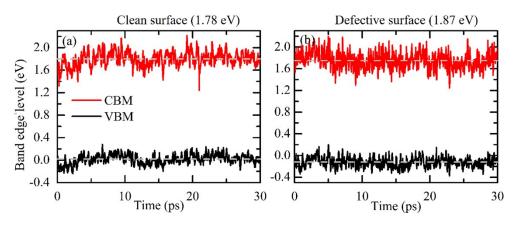


Fig. S2 Band edge level from AIMD simulation of MAI terminated with pristine-surface (left panel) and defect-surface (right panel). The gray dash line denotes the time averaged value of VBM and CBM.

^{*}Author to whom correspondence should be addressed. E-mail:

zilong.zheng@bjut.edu.cn, luyue@bjut.edu.cn