

Supporting Information

Atomic scale insight of adsorption and lateral interaction of F and O atoms on Al surfaces

Pengqi Hai^{1,2}, Chao Wu^{1,2*}, Xiangdong Ding^{2*}

1. Frontier Institute of Science and Technology, Xi'an Jiaotong University, Xi'an 710049, People's Republic of China;
2. State Key Laboratory for Mechanical Behavior of Materials, School of Materials Science and Engineering, Xi'an Jiaotong University, Xi'an 710049, People's Republic of China
E-mail: chaowu@mail.xjtu.edu.cn, dingxd@mail.xjtu.edu.cn

Table of Contents

Table S1 The interaction between O and F adatom used in CMC simulation on Al(111).....	S2
Figure S1. The most stable adsorption structures of F atom on Al surfaces.....	S3
Figure S2 Adsorption configurations of F atoms under different coverage on Al surface.....	S4
Figure S3. Average first-neighbor coordination numbers of O (0.05ML) and F (0.01ML) adatoms.....	S5
Figure S4. Snapshots of configurations after 40,000,000 at different temperatures.....	S6
Figure S5. The F and O percentage as function of height with coverage of 0.25 ML.....	S7
Figure S6. Snapshots of configurations at 0.56ML under different temperatures after running 400 ps.....	S8
Figure S7. Snapshots of configurations at 0.25ML under different temperatures after running 400 ps.....	S9

	O-O	O-F	F-F
Interaction (eV)	-0.11	-0.14	0.07

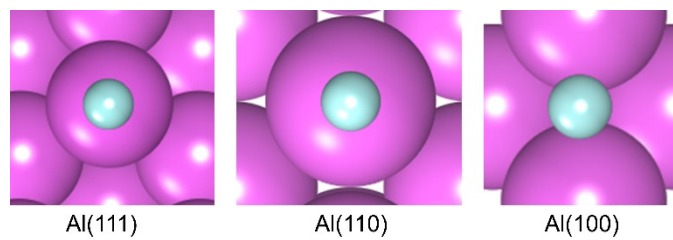


Figure S1. The most stable adsorption structures of F atom on Al surfaces.

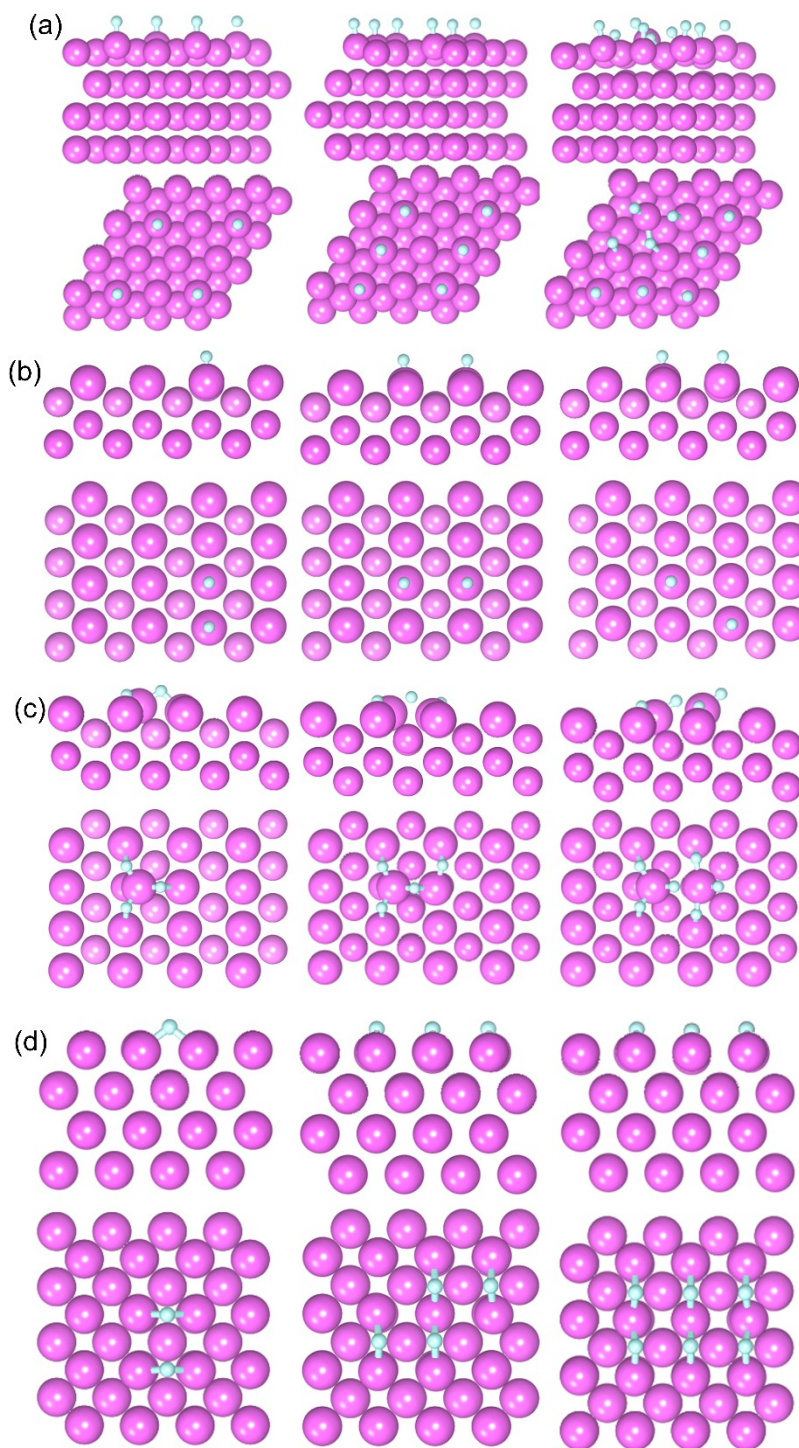


Figure S2. Adsorption configurations of F atoms under different coverage on Al surface. (a) Al(111), (b) and (c) Al(110), (d) Al(100). Pink, red and light blue ball represent Al and F atom, respectively.

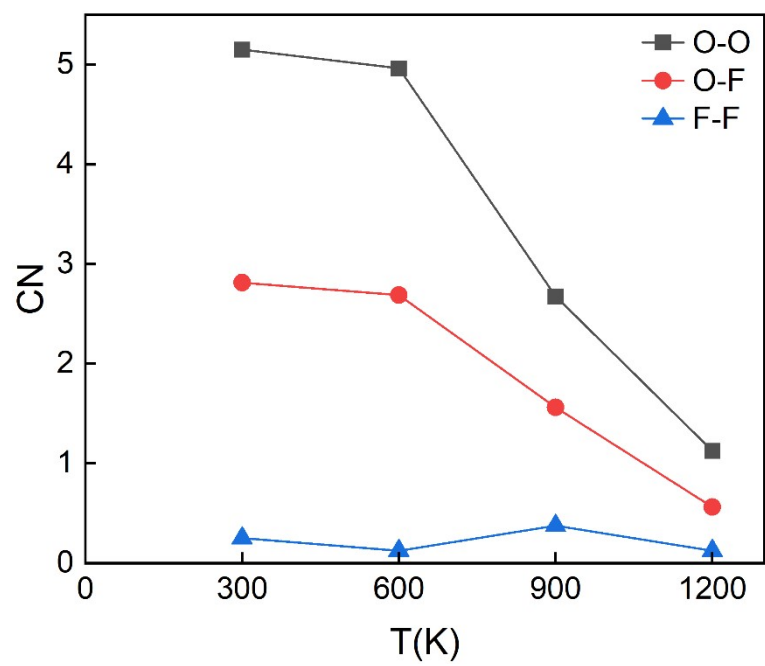


Figure S3. Average 1NN coordination numbers (CN) of O (0.05ML) and F (0.01ML) adatoms.

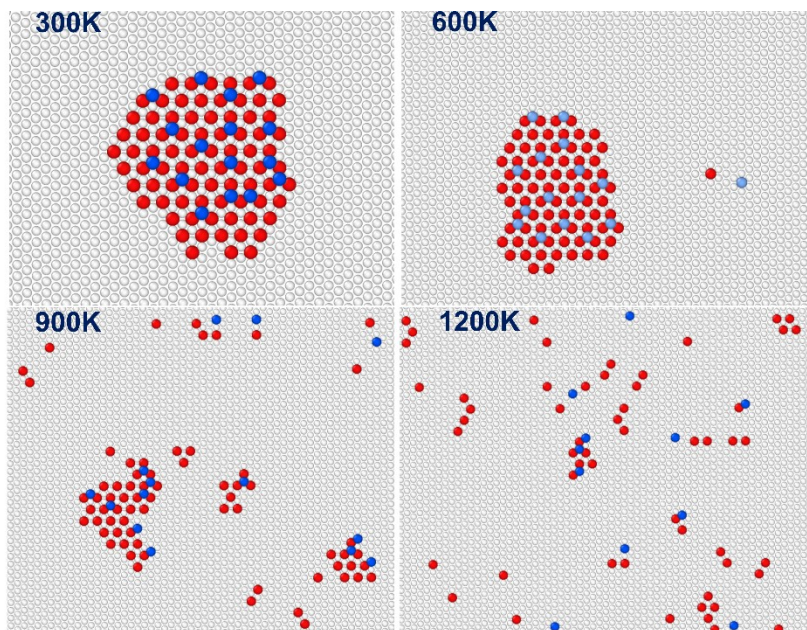


Figure S4. CMC snapshots of configurations after 40,000,000 steps at different temperatures.

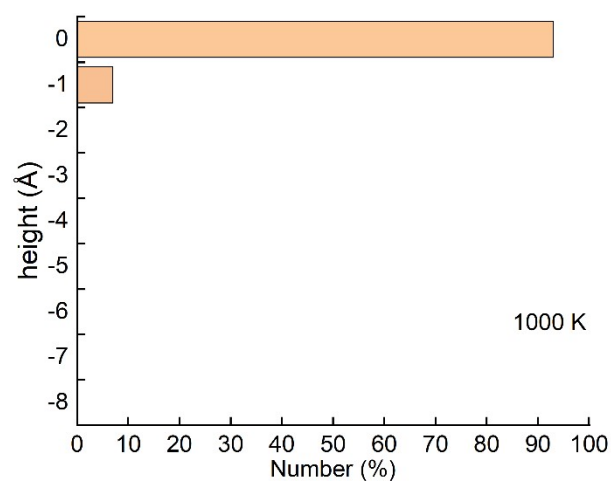
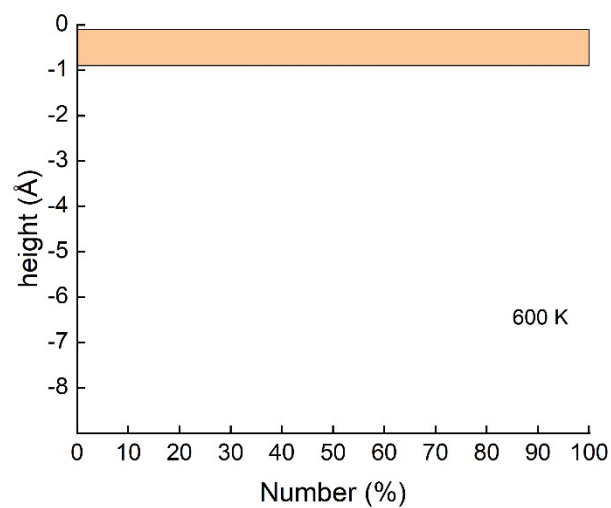
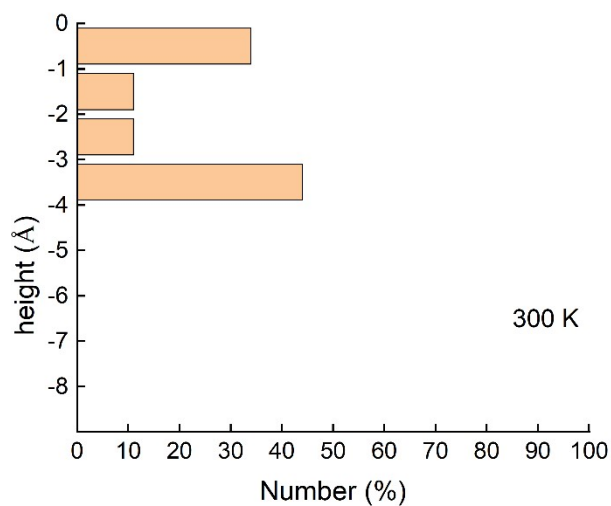


Figure S5. The F percentage as function of height under the O and F coverage of 0.25 ML at different temperatures.

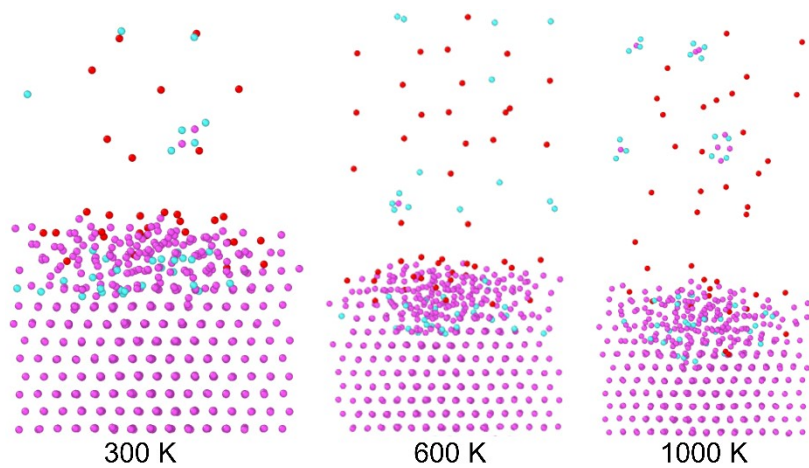


Figure S6. RMD snapshots of configurations at 0.56 ML under different temperatures after 400 ps.

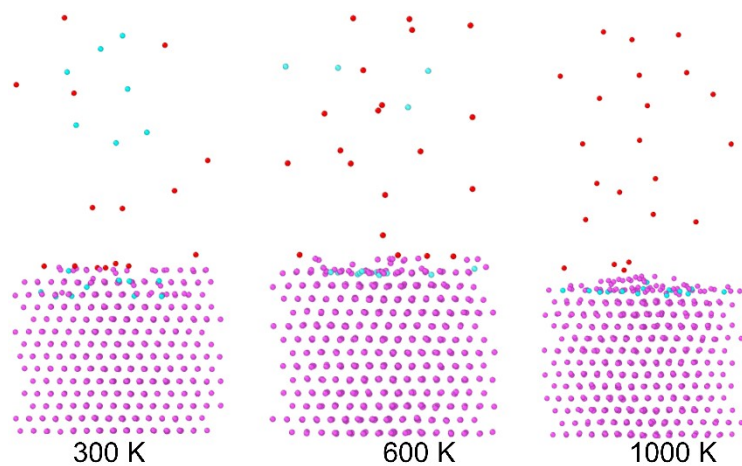


Figure S7. RMD snapshots of configurations at 0.25ML under different temperatures after 400 ps.