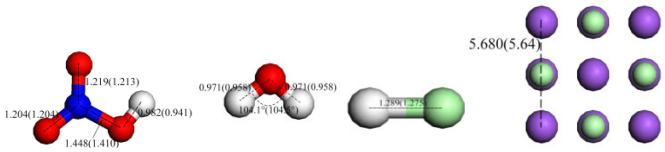
Supplementary material



HNO_3 H_2O HCl NaCl

Fig. S1 Optimized geometries for gaseous HNO_3, H_2O and HCl molecules as well as the bulk NaCl. The distances are in angstrom, and the angles are in degree. The values in parentheses are experimental data. Purple ball: Na; green ball: Cl; blue ball: N; red ball: O; white ball: H

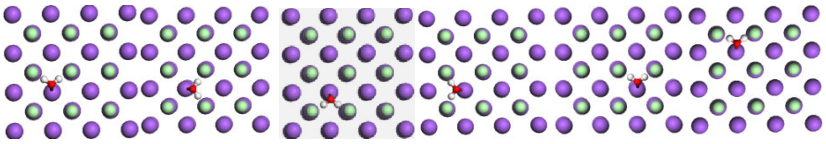
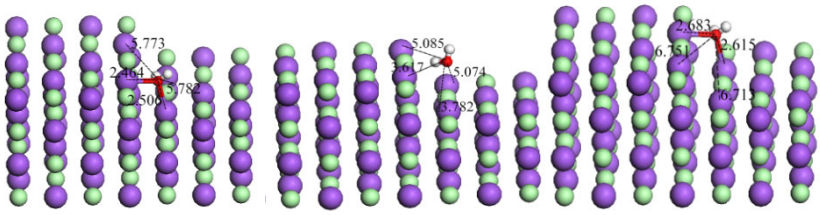
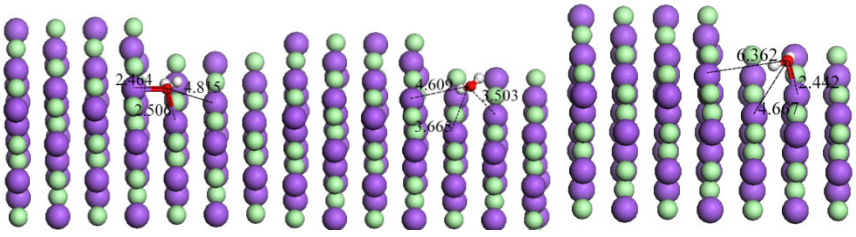


Fig. S2 Equivalent adsorption configurations of the water molecule on the NaCl (100) surface. Purple ball: Na; green ball: Cl; red ball: O; white ball: H



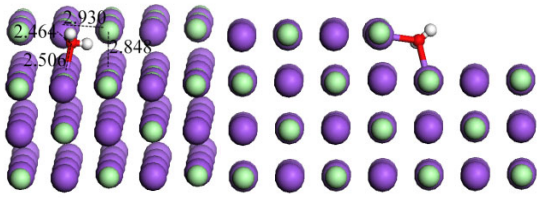
Before diffusion TS2 After diffusion

Fig. S3 Configuration of the transition state and the configurations before and after the water diffusion along the step on the stepped (710) surface. The distances are in angstrom. Purple ball: Na; green ball: Cl; red ball: O; white ball: H. TS2: the transition state

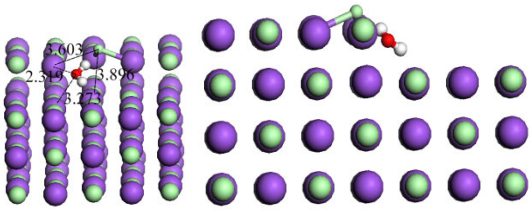


Before diffusion TS3 After diffusion

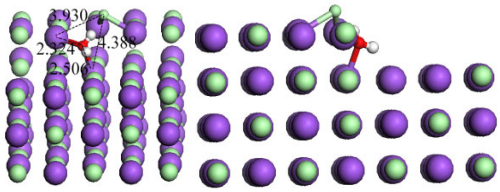
Fig. S4 Configuration of the transition state and the configurations before and after the water diffusion on stoichiometric (100)-like plane of the stepped (710) surface. The distances are in angstrom. Purple ball: Na; green ball: Cl; red ball: O; white ball: H. TS3: the transition state



Before the reconstruction (top view) Before the reconstruction (side view)



TS5 (top view) TS5 (side view)



After the reconstruction (top view) After the reconstruction (side view)

Fig. S5 Configuration of the transition state and the configurations before and after the surface reconstruction of the water-adsorbed (710) surface. The distances are in angstrom. Purple ball: Na; green ball: Cl; red ball: O; white ball: H. TS5: the transition state