

Description of Additional Supplementary Files

File Name: Supplementary Movie 1

Description: *Ab initio* molecular dynamics (AIMD) simulation of a model Si(111) surface with an isolated surface Au atom. An Au atom was placed on a Si site in the initial structure. 10 molecules each of HF and H₂O₂ were placed randomly on the (111) surface of Si. Total duration: 50 ps.

File Name: Supplementary Movie 2

Description: *Ab initio* molecular dynamics (AIMD) simulation of a model Si(111) surface. 10 molecules each of HF and H₂O₂ were placed randomly on the (111) surface of Si. Total duration: 50 ps.