

Description of Additional Supplementary Files

File Name: Supplementary Movie 1

Description: Ab initio molecular dynamics (AIMD) simulation showing the motion of a single water molecule on a hexagonal boron nitride (h-BN) monolayer supported on a Ni(111) surface. The top panel presents a side view, revealing the vertical fluctuations and adsorption geometry of the molecule relative to the surface. The bottom panel shows a top view, highlighting the lateral diffusion pathway. The movie illustrates not only translational motion but also the characteristic rotational and precessional dynamics of the water molecule as it traverses the h-BN/Ni(111) surface.

File Name: Supplementary Movie 2

Description: Ab initio molecular dynamics simulation of a single water molecule on hBN/Ni(111). The top panel shows a side view, illustrating the adsorption geometry and vertical motion. The bottom panel shows a top view, capturing the molecule's lateral diffusion along with its rotational and precessional dynamics.

File Name: Supplementary Movie 3

Description: Ab initio molecular dynamics simulation of a single water molecule on hBN/Ni(111). The top panel shows a side view, illustrating the adsorption geometry and vertical motion. The bottom panel shows a top view, capturing the molecule's lateral diffusion along with its rotational and precessional dynamics.