

## Description of Additional Supplementary Files

File Name: Supplementary Dataset 1

Description: The supplementary dataset contains all relevant frequencies and adsorption energies used in generating the figures in the main article and supplementary information. The supplementary dataset includes frequency and energy data for  $O_2$ , OHx, NHx, CHx, and  $CH_2$  $CH_3$  species on the (111), (100), and (110) planes of Ag, Au, Cu, Ir, Pd, Pt, Ni and Rh.