

Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: Atomic coordinates for the computational models of electronic structure, including X-X-Qv1, X-Y-Qv1, X-X-Qv2, X-Y-Qv2, X-X-Qv3, X-Y-Qv3, X-X-Qv4, and X-Y-Qv4. The atomic coordinates for the computational models when adsorbing intermediates are also included.