DFT calculation performed

504 HEA sites
5 pure metals

504 HEA sites
0 pure metals

504 HEA sites
5 pure metals

27 HEA sites
5 pure metals

M-O bond is most pronounced when Cu is a neighbor
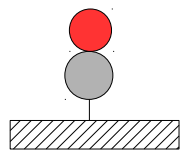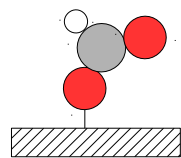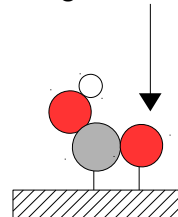

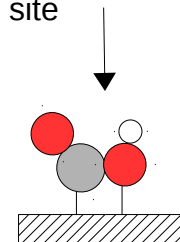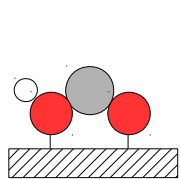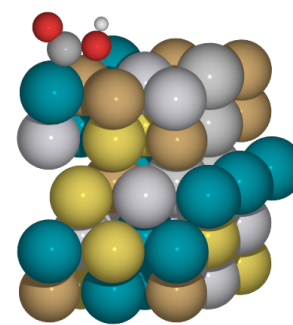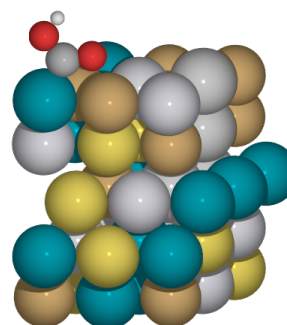26 HEA sites
5 pure metals

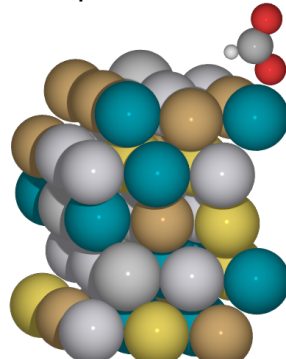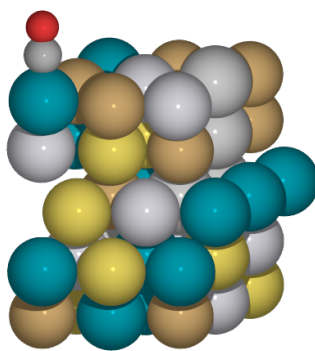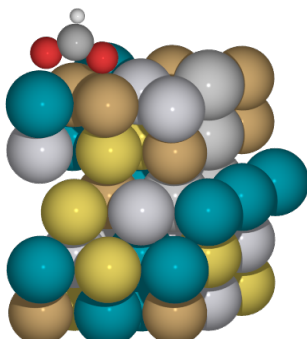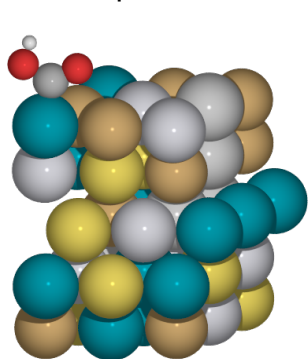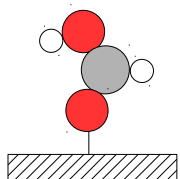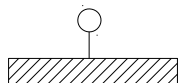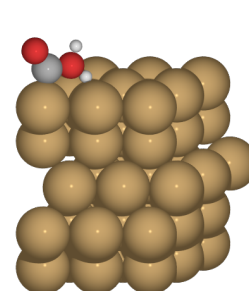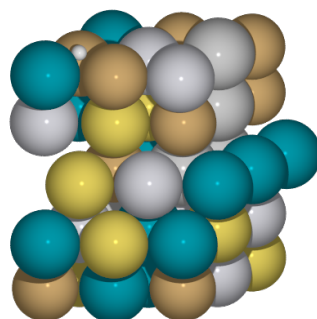M-O bond is most pronounced on a Cu-Cu site

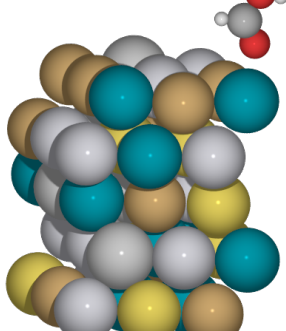26 HEA sites
5 pure metals
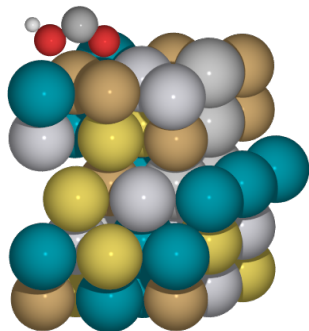

504 HEA sites
5 pure metals
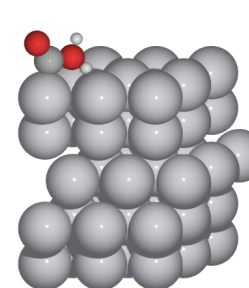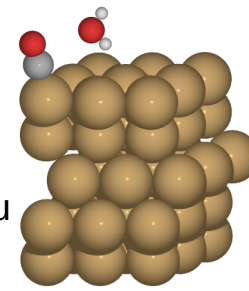

27 HEA sites
5 pure metals

490 HEA sites
5 pure metals

… hundreds of *OH and *O energies on 2x2x5 slabs

Ag/Au/Cu

Pt/Pd