

Figure S1. Structures of intermediates and transition states (TS) involved in the methanol synthesis reaction on the Cu<sub>29</sub> nanoparticle (Big brown: Cu; small white: H; small red: O; small grey: C)

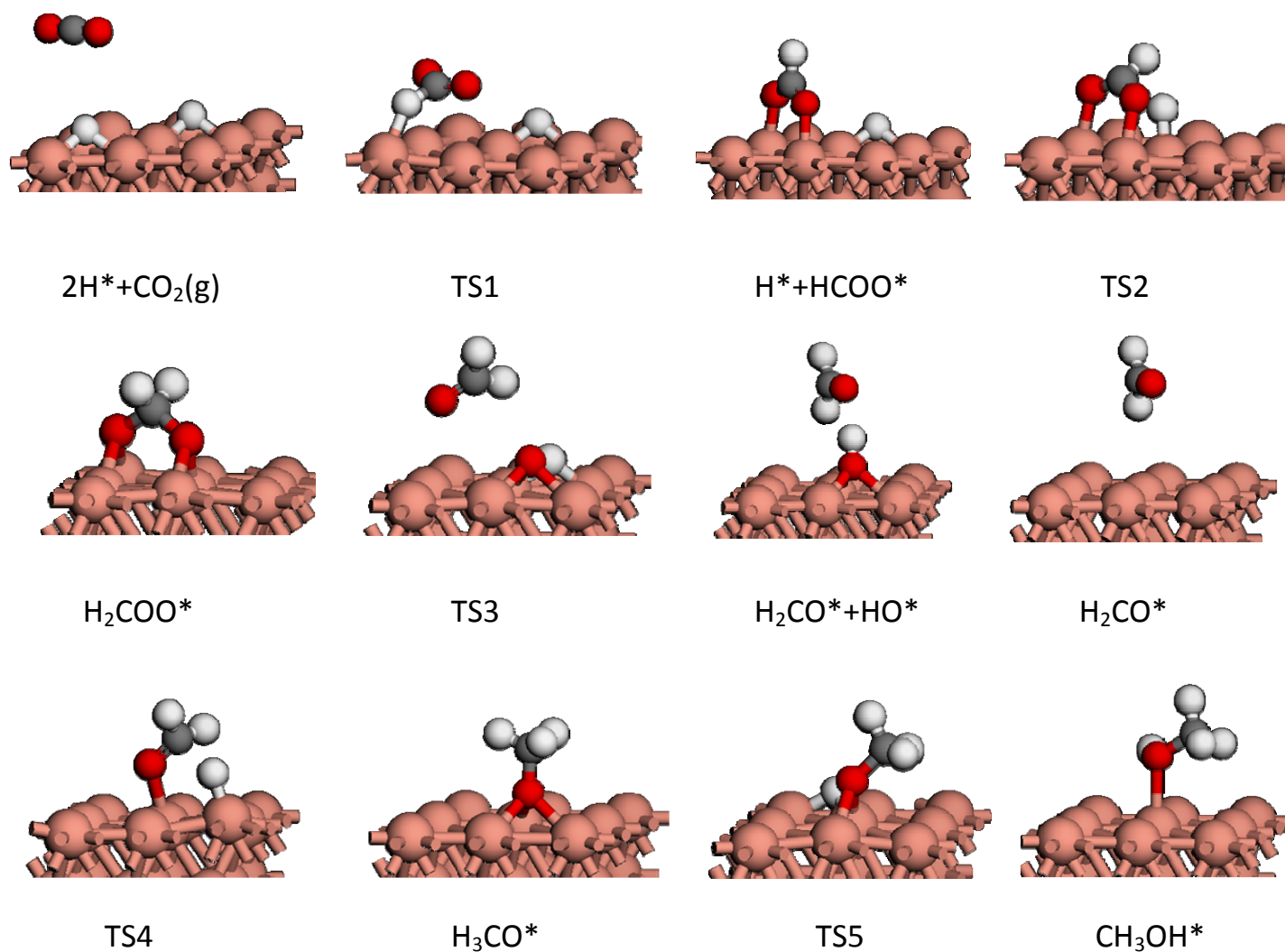


FIG. S2. Structures of intermediates and transition states (TS) involved in the methanol synthesis reaction on the Cu(111) surface (Big brown: Cu; small white: H; small red: O; small grey: C)