Supporting Information for

"Theoretical study of CO adsorption and activation on orthorhombic $Fe_7C_3(001)$ surfaces for Fischer–Tropsch synthesis using density functional theory calculations"

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1. $Fe_7C_3(001)$ slabs

Here, images of o-$Fe_7C_3(001)_{0.85}$, $(001)_{0.20}$, and $(001)_{0.99}$ are provided as representatives to show the fixed and unfixed atoms in the slab. The orange and gray balls in the figure represent Fe and C, respectively.

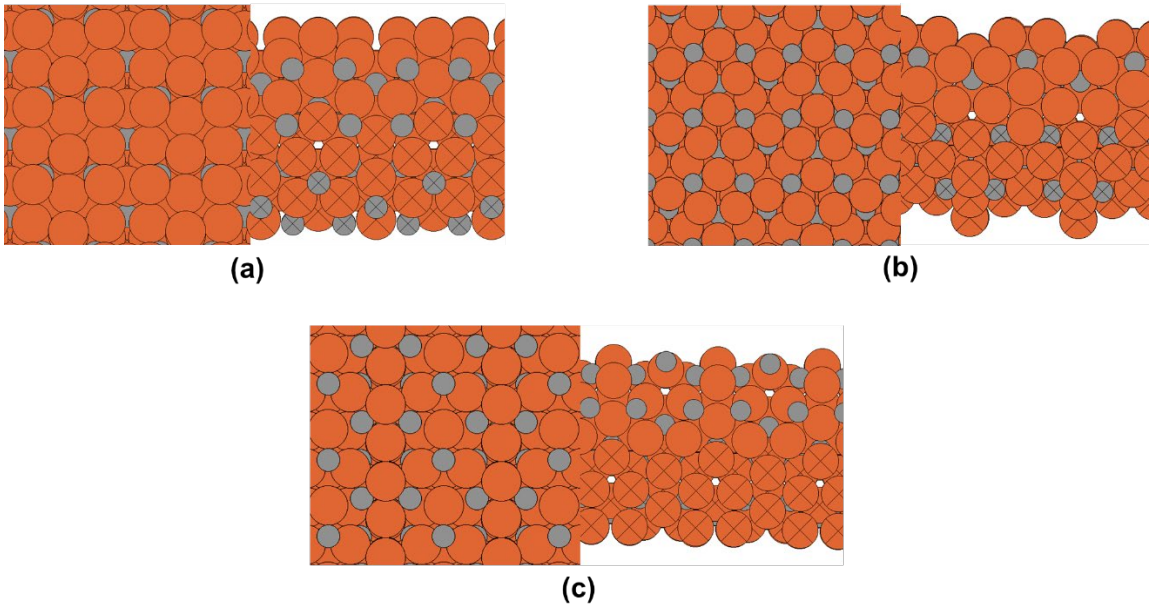

Figure S1. Top and side views of (a) o-$Fe_7C_3(001)_{0.85}$, (b) $(001)_{0.20}$, and (c) $(001)_{0.99}$ surfaces

2. Molecular configurations of CO* and C*

The orange, gray, and red balls in the figures represent Fe, C, and O, respectively.

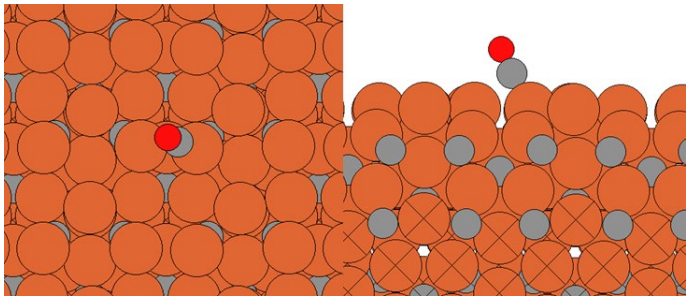

Figure S2. Top and side views of vertical CO* on o-$Fe_7C_3(001)_{0.85}$ surface

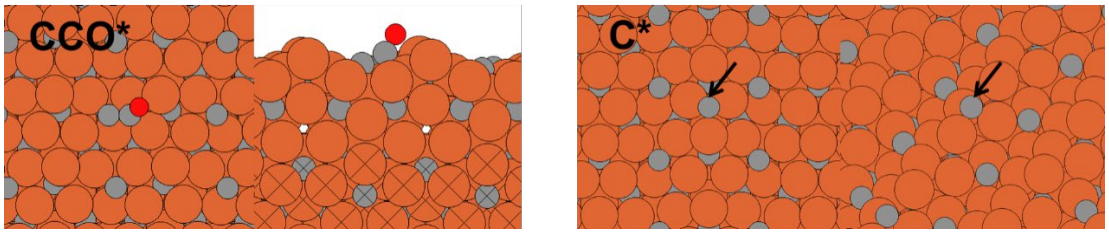

Figure S3. Top and side or angled views of CCO* and C* on o-$Fe_7C_3(001)_{0.13}$ surface

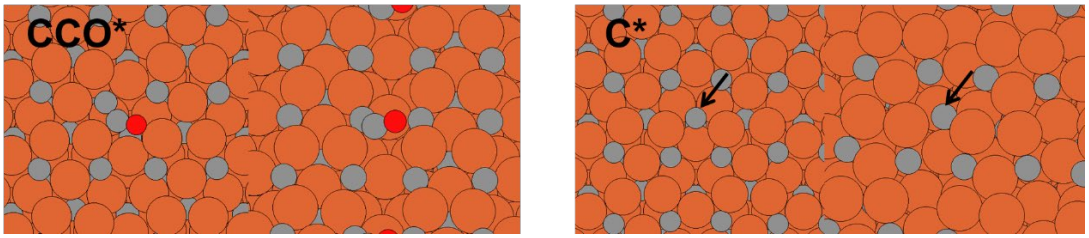

Figure S4. Top and side or angled views of CCO* and C* on o-$Fe_7C_3(001)_{0.20}$ surface

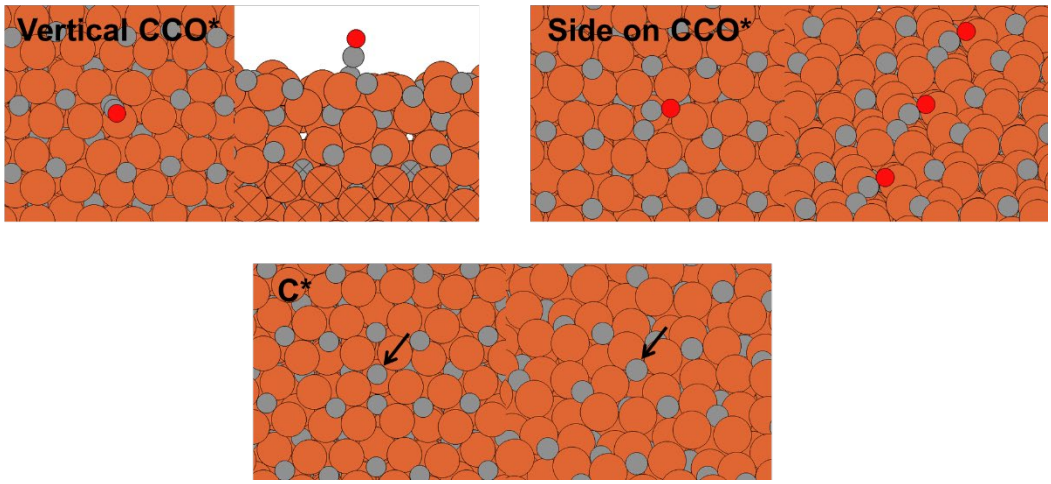

Figure S5. Top and side or angled views of vertical CCO*, side-on CCO*, and C* on o-$Fe_7C_3(001)_{0.09}$ surface

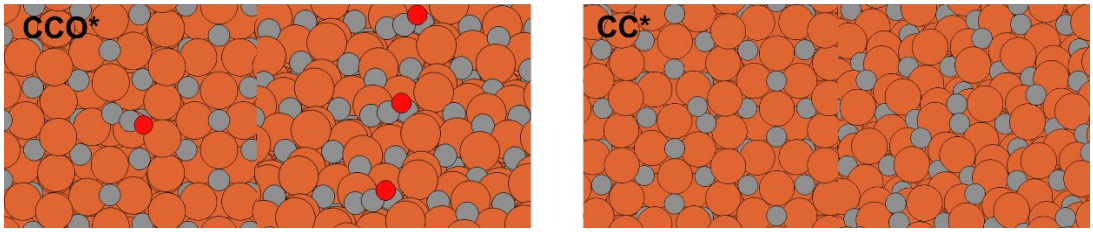

Figure S6. Top and side or angled views of CCO* and CC* on o-$Fe_7C_3(001)_{0.99}$ surface