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Hydrogen-assisted versus Hydroxyl-assisted CO Dissociation over Co-doped Cu(111): a DFT Study

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Highlights

- The first comprehensive DFT study of OH-assisted CO hydrogenation reactions on Co-doped Cu(111) surface was done.
- The first overall comparison study of activation barrier between H-assisted and OH-assisted hydrogenation routes was done.
- The change of C-O bond and adsorption of carbon intermediates when co-adsorbed with H atom, OH molecule and O atom were discussed.

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