

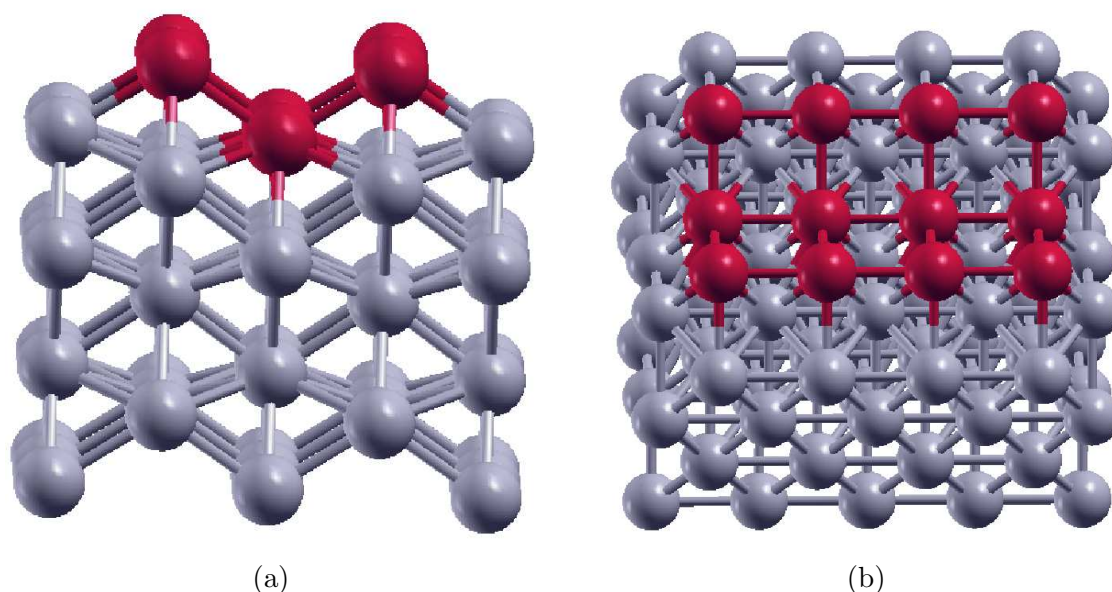


Figure S1: The hcp ($10\bar{1}0$) B surface slab with eight layers, (a) lateral view and (b) top view. The six-fold (F_6) active sites for CO dissociation are shown in red color.

Model and Computational Details

The present calculations have been performed using the periodic density functional theory approach based on the plane wave basis set as implemented in the VASP code.¹ The core potential has been described by the projected augmented wave (PAW) method.² The exchange-correlation functional is expressed by the the generalized-gradient approximation (GGA) with Perdew-Becke-Erzenhof (PBE) functional.³

In the present work we use the Ru and Co surfaces corresponding to a ($10\bar{1}0$)B surface. The surface has been modeled using a 2×2 super-cell consisting of an 8 layered slab and 10 layers of vacuum between the slabs. The k-point sampling was generated following the Monkhorst-Pack procedure with a $5\times 5\times 1$ mesh. The energy cut-off used for the plane wave was 400 eV. In the case of Co surface we do spin polarized calculations. The optimization has been carried out using the conjugate gradient technique. The reaction paths have been generated by the nudged elastic band (NEB) as implemented in VASP.⁴ It should be noted that all the atoms of the slab have been relaxed during the optimization and NEB calculations. The transition states have been confirmed by the saddle points obtained from the frequency calculations. The ($10\bar{1}0$)B surface is shown in Fig. 1. The active six-fold sites (F_6) are shown in red color. The optimized lattice constants used for Ru and Co were

2.69 and 2.50 Å respectively in agreement with the experimental data.⁵

Table S1: The C–O, H–C and HC–O bond lengths in Å for the initial (IS), transition (TS) and final (FS) states on Ru (10 $\bar{1}$ 0)B and Co(10 $\bar{1}$ 0)B surfaces.

Reactions	Ru(10 $\bar{1}$ 0)B			Co(10 $\bar{1}$ 0)B		
	IS	TS	FS	IS	TS	FS
CO + H $\longrightarrow$ C + O + H	1.37	1.85	3.56	1.34	2.04	3.46
CO + H $\longrightarrow$ HCO	2.58	1.51	1.23	2.62	1.53	1.21
HCO $\longrightarrow$ CH + O				1.38	1.89	3.13

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