

The Conversion of CO₂ to Methanol on orthorhombic β -Mo₂C and Cu/ β -Mo₂C Catalysts: Mechanism for Admetal Induced Change in the Selectivity and Activity

Sergio Posada-Pérez,^a Pedro J. Ramírez,^b Ramón A. Gutiérrez,^b Dario J. Stacchiola,^c Francesc Viñes,^{a,*} Ping Liu,^c Francesc Illas^a and José A. Rodríguez^{c,*}

^a *Departament de Química Física & Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, c/ Martí i Franquès 1, 08028 Barcelona, Spain*

^b *Facultad de Ciencias, Universidad Central de Venezuela, Caracas 1020-A, Venezuela*

^c *Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973, USA*

*Corresponding authors: francesc.vines@ub.edu; rodriguez@bnl.gov

Figure S1. Energy profile of CO₂ hydrogenation *via* HCOOH formation as predicted from a Cu₄/β-Mo surface model

