Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

SUPPORTING INFORMATION

Direct Deoxygenation Reaction of Biomass Pyrolysis Oxygenated Model Compounds on Ni_5P_4(001) surface: Computational Study

Omer Elmutasim[1,2], Kyriaki Polychronopoulou[1,2,*]

[1]*Mechanical Engineering Department, Khalifa University, P.O. Box 127788, Abu Dhabi, United Arab Emirates.*

[2]*Center for Catalysis and Separation (CeCaS), Khalifa University, P.O. Box 127788, Abu Dhabi, United Arab Emirates*.

*Corresponding author email: kyriaki.polychrono@ku.ac.ae

Table S1: Bader charges (Q, in |e|) for a phenol molecule in the gas phase $(C_6H_6O)_{gas}$ and molecularly adsorbed (C_6H_6O/Ni_5P_4) on Ni_5P_4 surface. Bader charge differences($C_6H_6O/Ni_5P_4 - (C_6H_6O)_{gas}$) are also tabulated.

Atom	Gas-phase C_6H_6O	C_6H_6O/Ni_5P_4	$C_6H_6O/Ni_5P_4 - (C_6H_6O)_{gas}$
C	5.99	6.08	0.09
C	5.98	6.22	0.24
C	6.08	6.03	-0.05
C	6.06	6.10	0.04
C	5.48	5.50	0.02
C	6.00	6.14	0.13

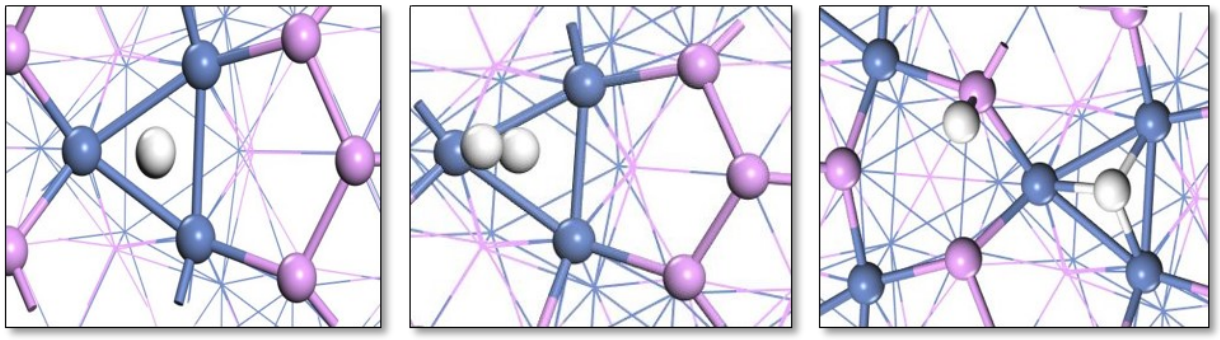
H	0.97	0.87	-0.09
H	0.88	0.92	0.04
H	0.92	0.92	0.00
H	0.96	0.91	-0.05
H	0.91	0.91	0.00
H	0.33	1.29	0.97
O	9.12	9.20	0.08
Total	**49.68**	**51.09**	**1.41**

Table S2: Bader charges (Q, in |e|) for a guaiacol molecule in the gas phase $(C_7H_8O_2)_{gas}$ and molecularly adsorbed ($C_7H_8O_2/Ni_5P_4$) on Ni_5P_4 surface. Bader charge differences($C_7H_8O_2/Ni_5P_4 - (C_7H_8O_2)_{gas}$) are also tabulated.

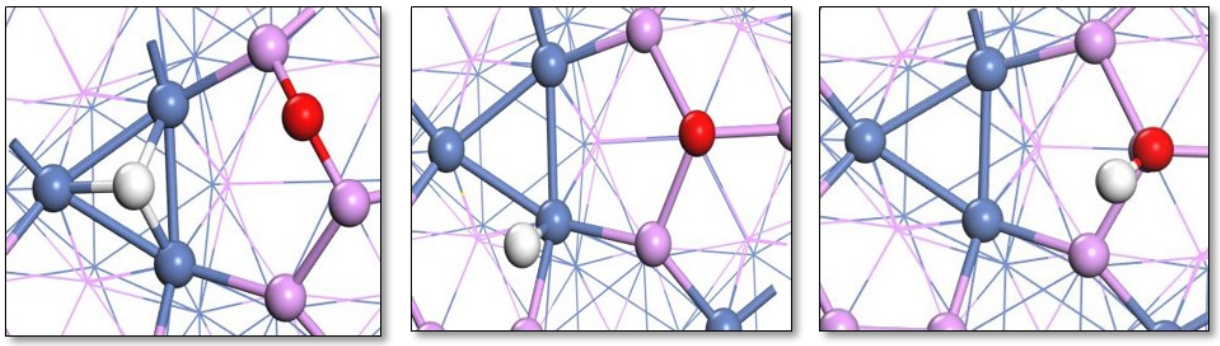
Atom	**Gas-phase** $(C_7H_8O_2)_{gas}$	$C_7H_8O_2/Ni_5P_4$	$C_7H_8O_2/Ni_5P_4 - (C_7H_8O_2)_{gas}$
C	6.03	6.09	0.06
C	6.12	6.04	-0.09
C	6.03	6.08	0.05
C	5.49	5.46	-0.03
C	5.51	5.54	0.04
C	6.01	6.13	0.12
C	5.66	6.13	0.47
H	0.94	0.92	-0.02
H	0.96	0.87	-0.09
H	0.90	0.87	-0.03
H	0.88	0.96	0.07
H	0.32	0.34	0.02
H	0.93	0.88	-0.05
H	0.90	0.89	-0.01
H	0.91	1.34	0.43

O	9.26	9.43	0.17
O	9.07	9.13	0.06
Total	**65.94**	**67.09**	**1.16**

a) R1



b) R5



c) R6

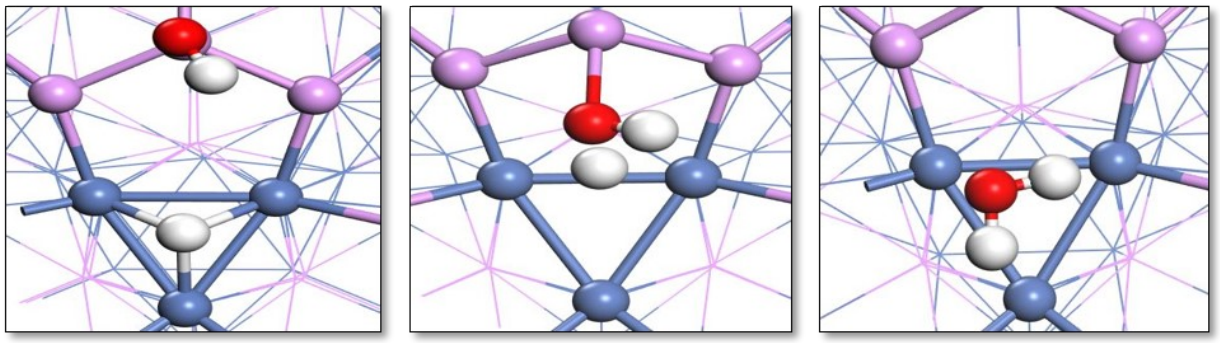


Figure S1: Top and side views of the initial state structure (left), the transition state (middle) and final state (right) for elementary steps R1, R5 and R6 related to Phenol DDO reaction on $Ni_5P_4(\bar{0}01)$ surface; (Ni: blue; P: purple; C: black; O: red; and H: white).

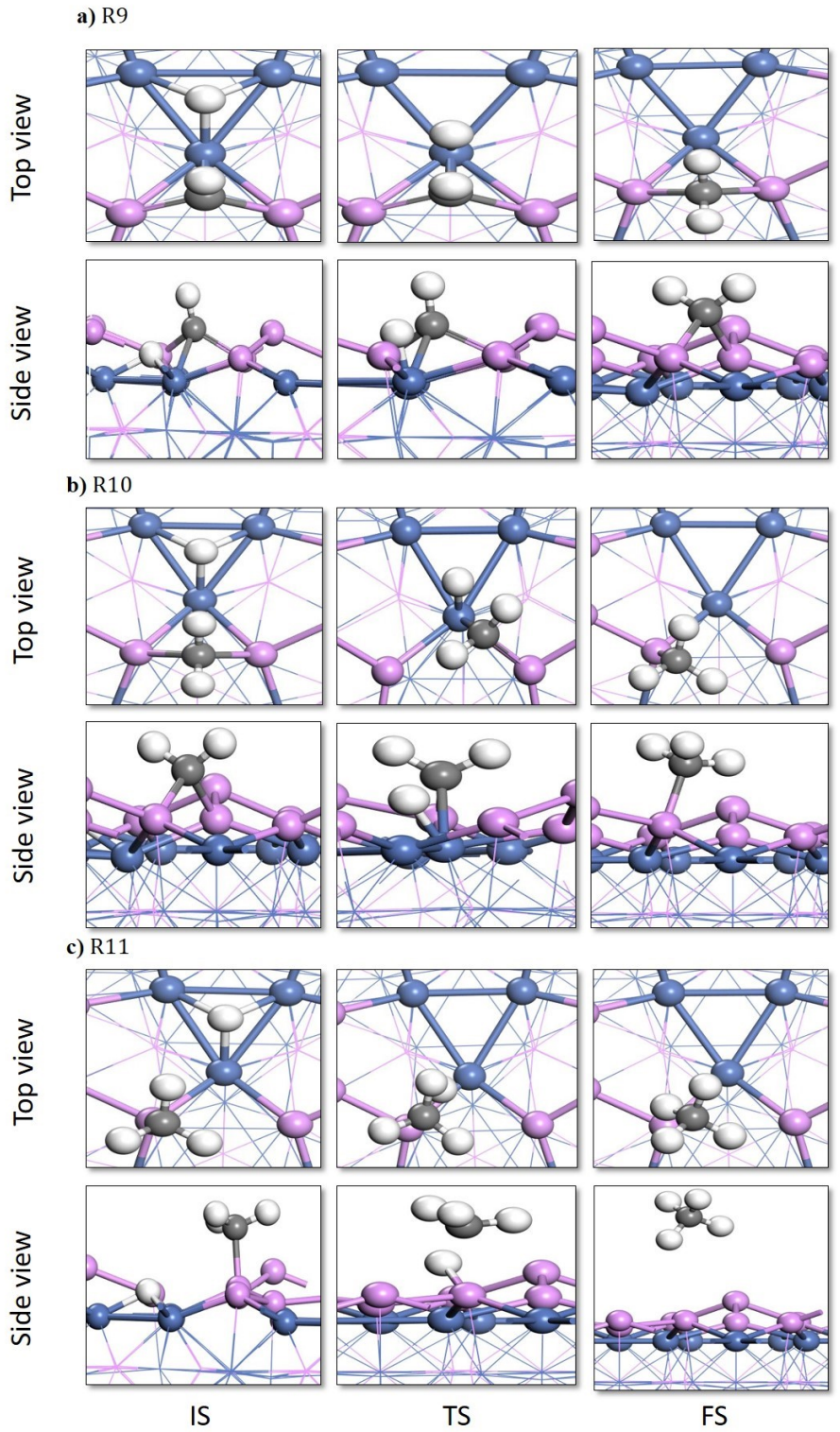


Figure S2: Top and side views of the initial state structure (left), the transition state (middle) and final state (right) for elementary steps R8, R9 and R10 pertained to CH_4 formation on $Ni_5P_4(001)$surface; (Ni: blue; P: purple; C: black and H: white).

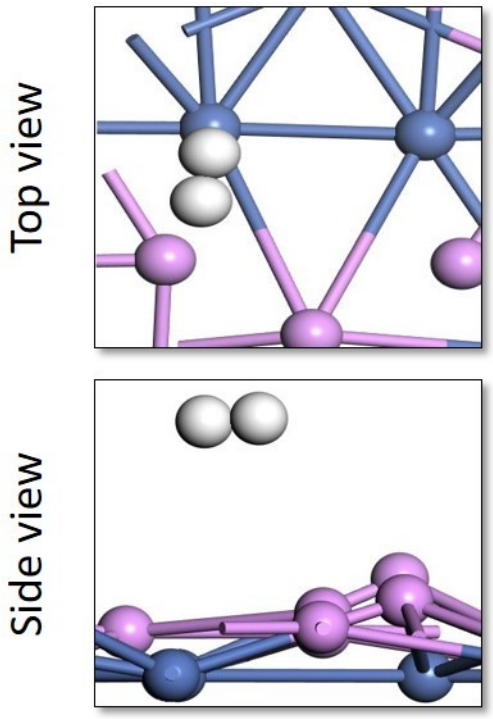


Figure S3: Top and side views of H_2 molecule physisorbed at Ni-P bridge site on $Ni_5P_4(001)$ surface; (Ni: blue; P: purple; C: black; O: red; and H: white).