

Supplementary information  
for  
From Digital Blueprint to Chemical Reality: Methanol  
to Formaldehyde at Ambient Conditions

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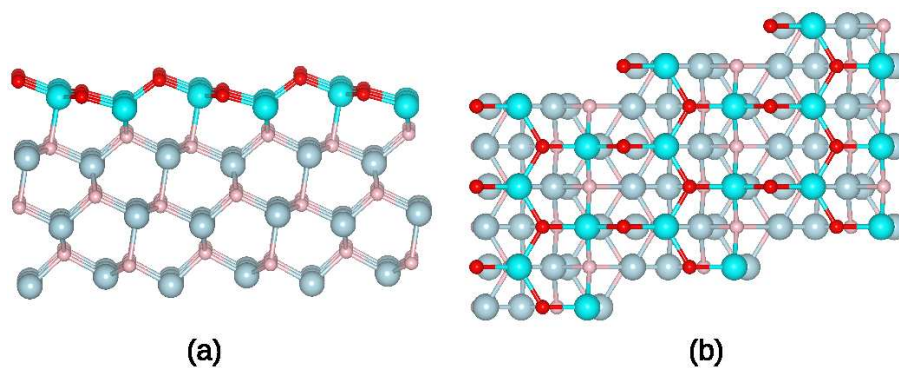


Figure 1: Structural geometry of  $(10\bar{1}1)$  facet of ZnO. (a) shows the side view. (b) shows the top view.

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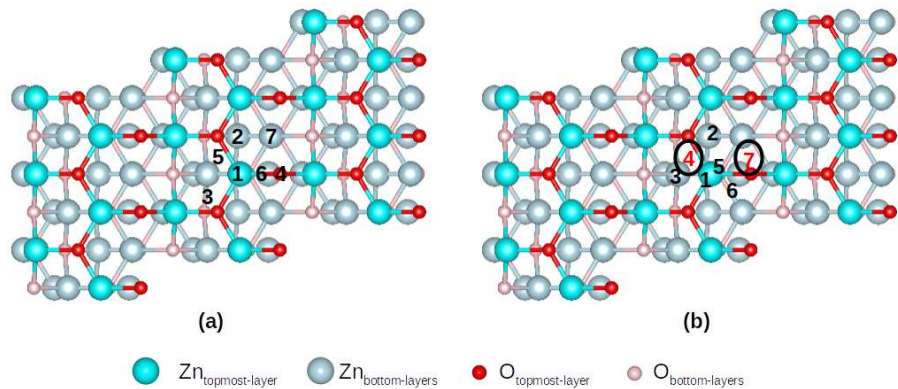


Figure 2: (a) schematic representation of initial positions where MeOH is placed on  $(10\bar{1}1)$  facet and (b) the positions where it adsorbed/dissociated after optimization. The numbers in black denote molecular adsorption while dissociation is shown in red color enclosed in black circle.

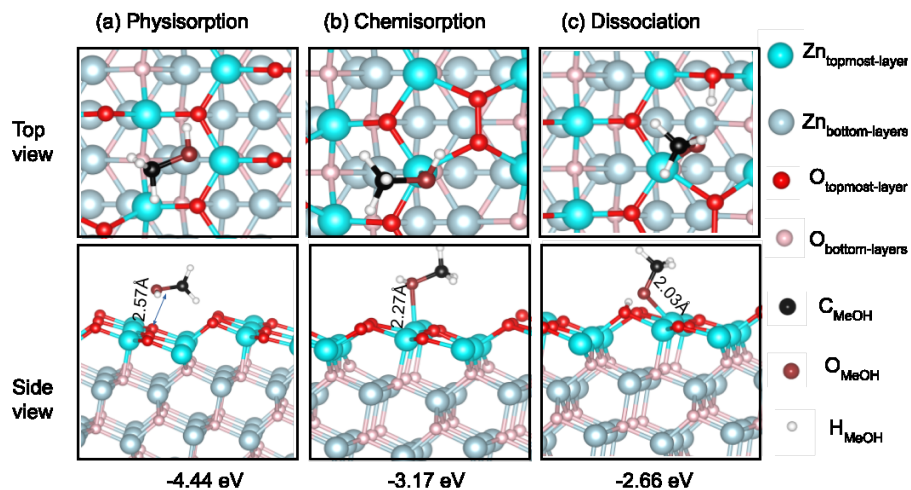


Figure 3: Methanol adsorbed at ZnO  $(10\bar{1}1)$  facet. (a) represents physisorption of MeOH at the ZnO  $(10\bar{1}1)$  surface. (b) shows the chemisorption of methanol at ZnO surface. (c) shows the dissociation of methanol at the ZnO facet. The methoxy group adsorbs at the Zn site, while the H adsorbs at  $O_{surf}$  site.

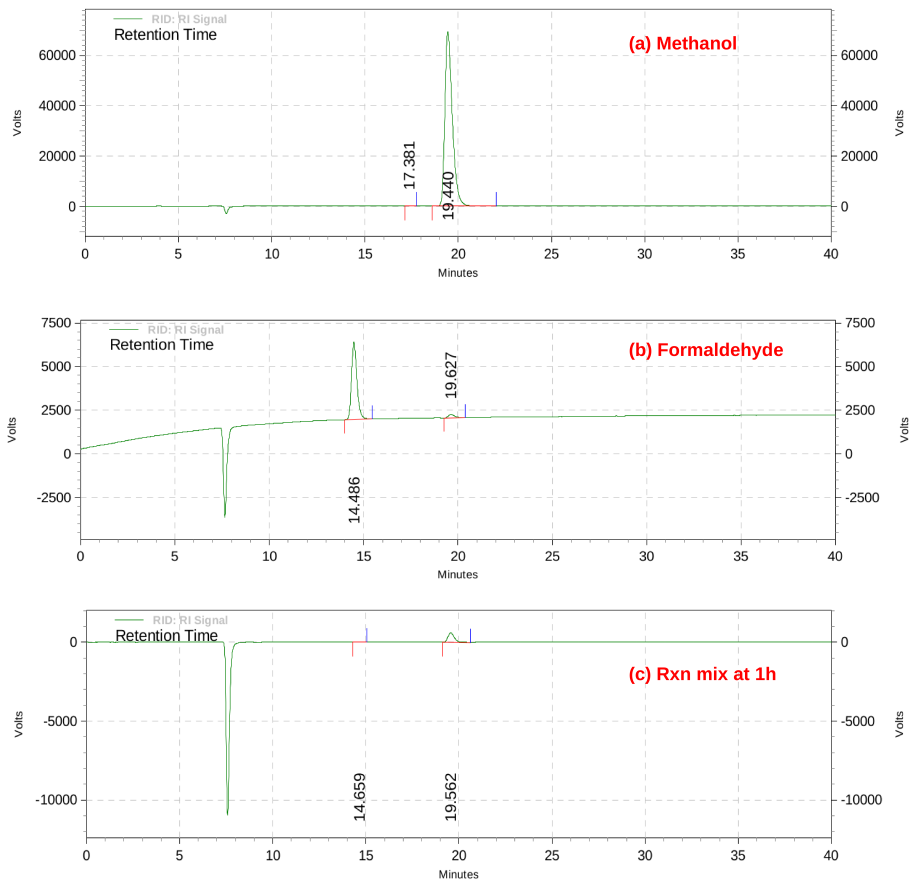


Figure 4: HPLC results for authentic samples with the known concentration of (a) methanol, and (b) formaldehyde. (c) HPLC result recorded for reaction mixture with ZnO catalyst at 1 h. The results show only two peaks of methanol (reactant) and formaldehyde (product) signify 100% selectivity.