

Supporting Information

Insights into the effect of Pt dopant into Cu(110)/H₂O for methanol

decomposition: A density functional theory study

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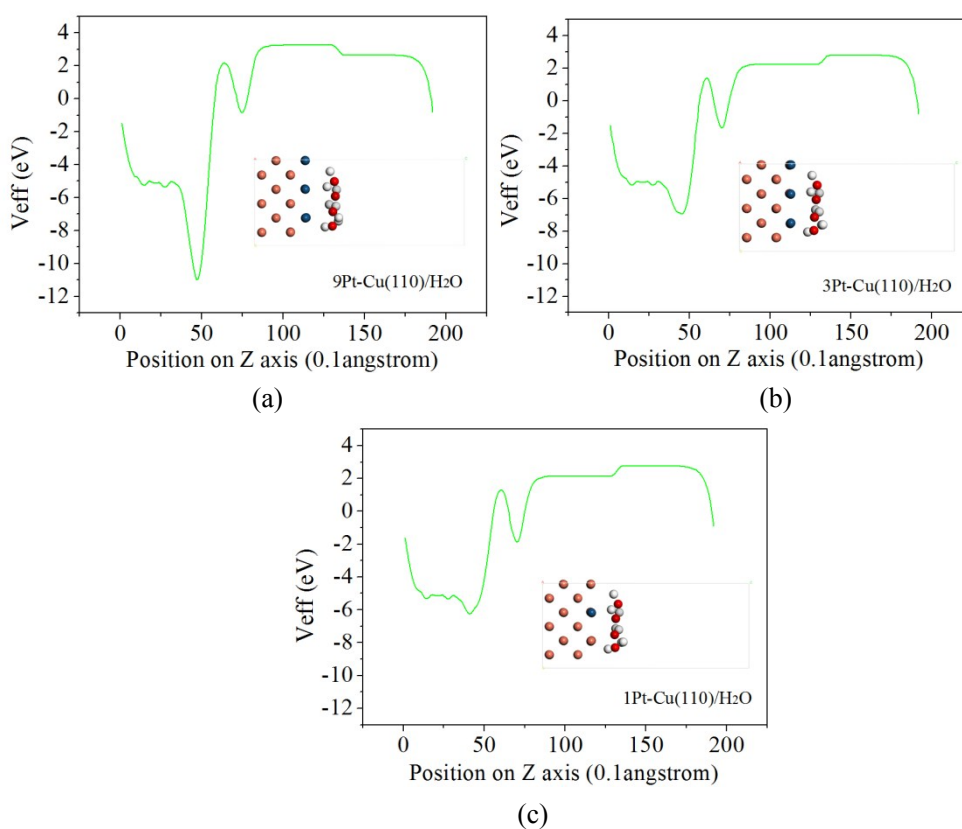


Fig.S1 The average electrostatic potential through the slab of the Z axis direction, (a) 9Pt-Cu(110)/H₂O, (b) 3Pt-Cu(110)/H₂O and (c) 1Pt-Cu(110)/H₂O.

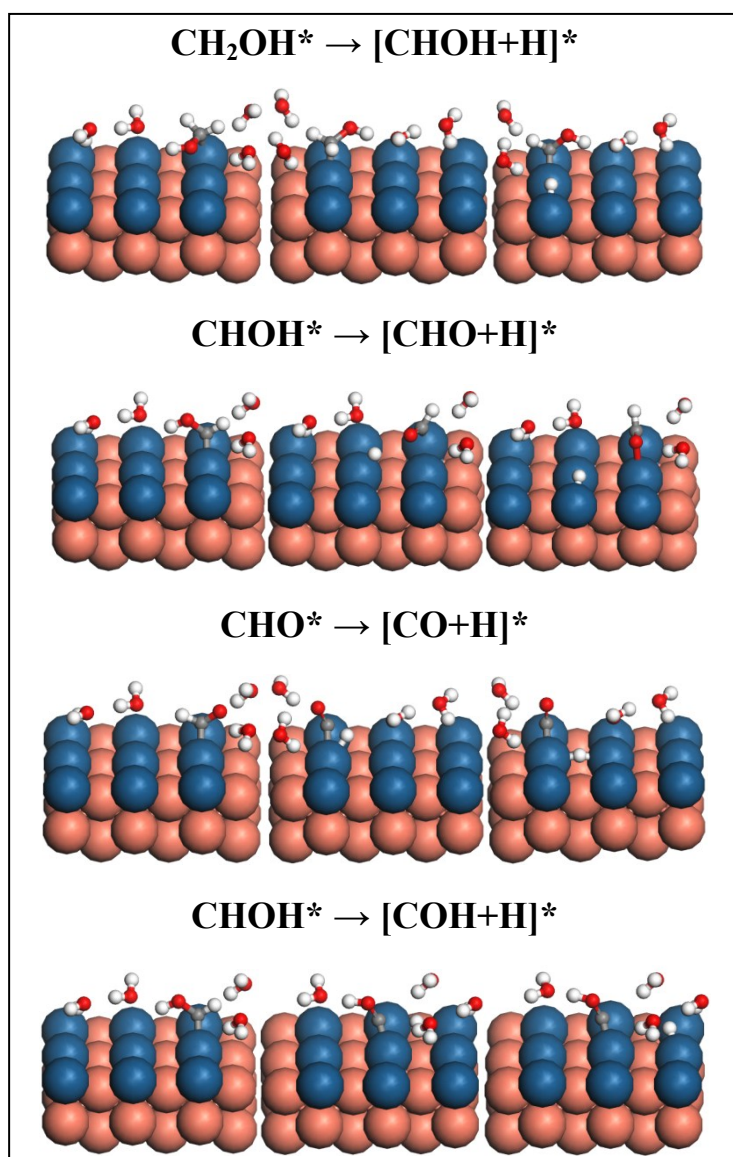


Fig.S2 Schematic representation of the C-H bond breaking route of CHOH for the methanol decomposition on 9Pt-Cu(110)/H₂O surface. Cu, Pt, C, O and H atoms are shown in brown, blue, gray, red and white spheres, respectively.

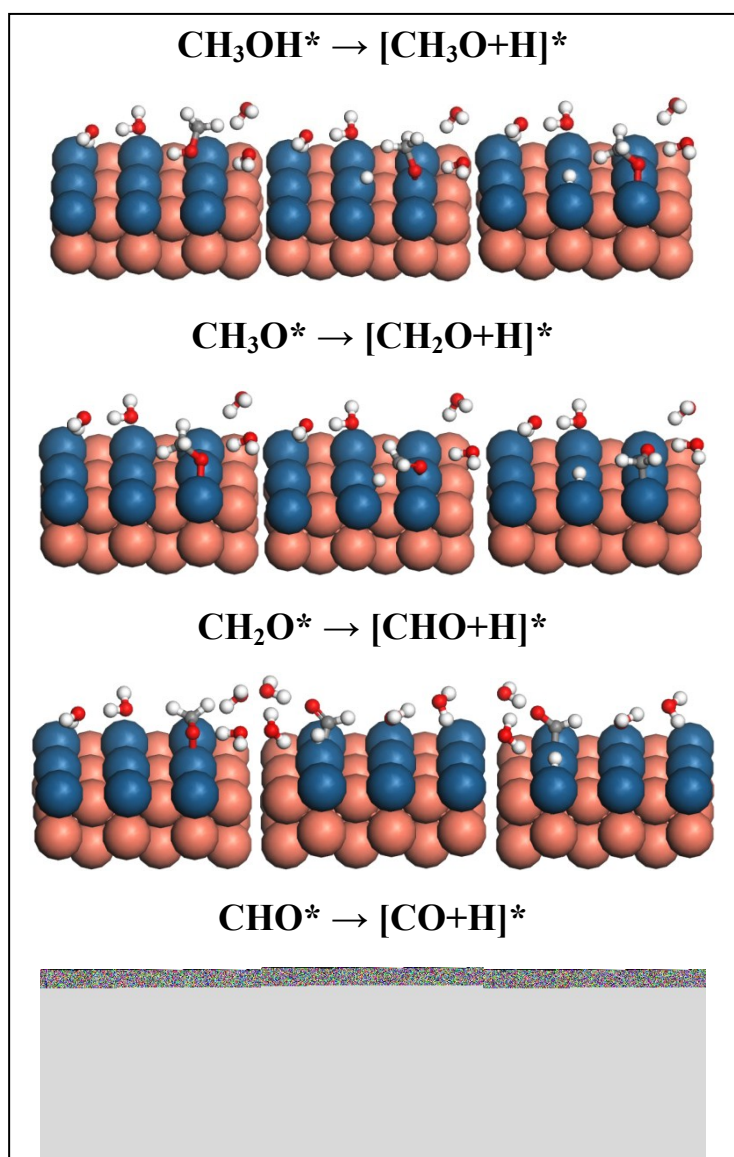


Fig.S3 Schematic representation of the O-H bond breaking route for the methanol decomposition on 9Pt-Cu(110)/H₂O surface. See Fig.S2 for color coding.

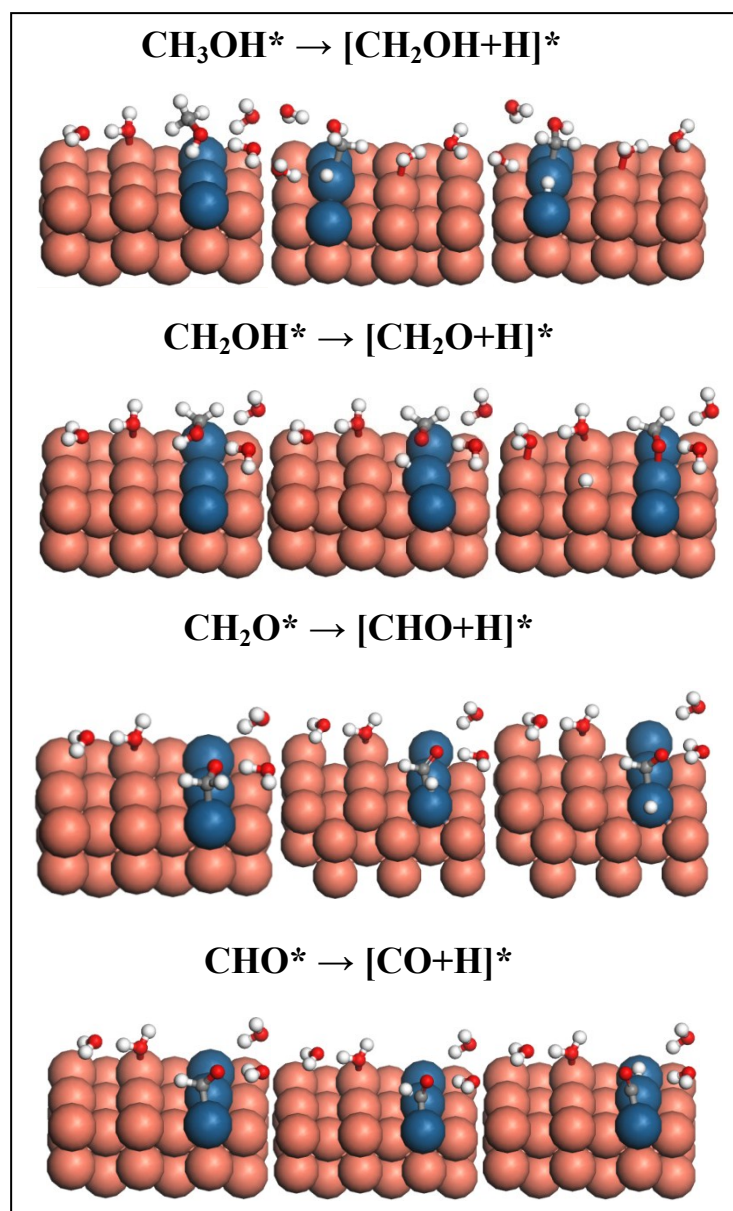


Fig.S4 Schematic representation of the C-H bond breaking route for the methanol decomposition on 3Pt-Cu(110)/H₂O surface. See Fig.S2 for color coding.

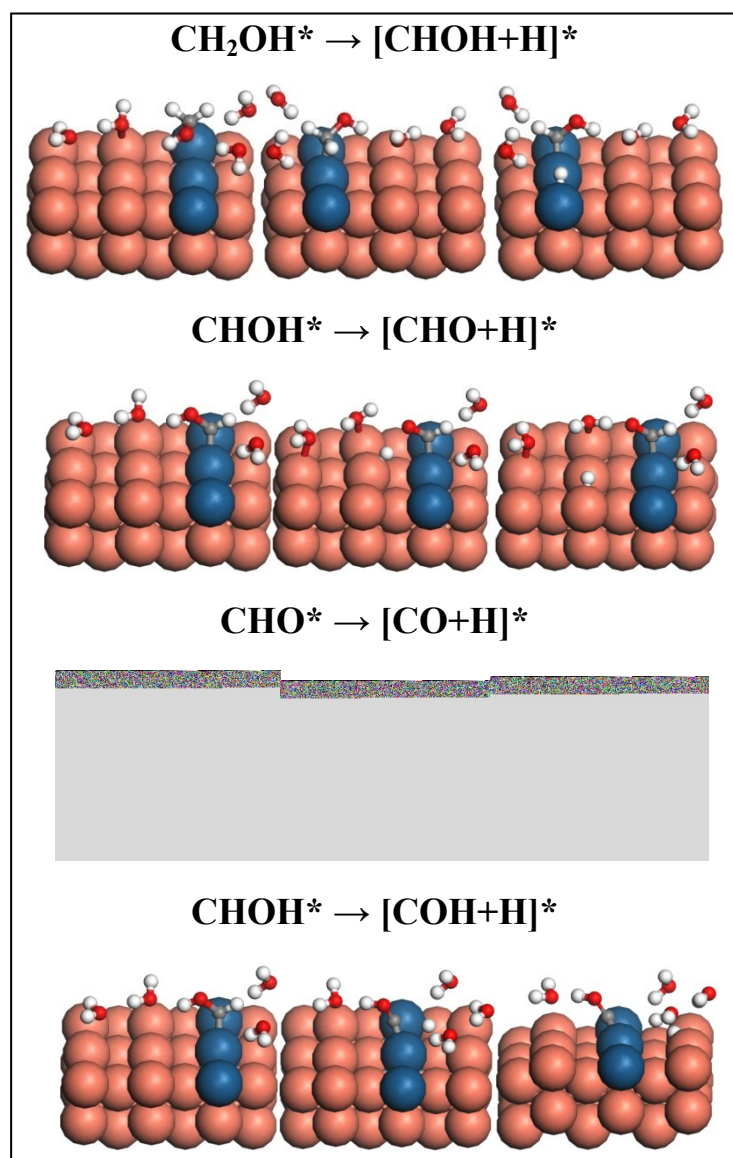


Fig.S5 Schematic representation of the C-H bond breaking route of CHOH for the methanol decomposition on 3Pt-Cu(110)/H₂O surface. See Fig.S2 for color coding.

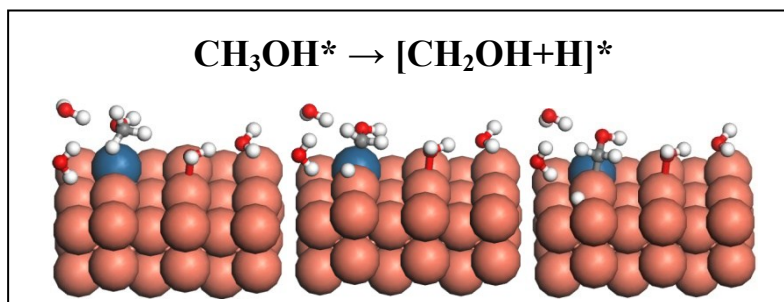


Fig.S6 Schematic representation of the C-H bond breaking route for the methanol decomposition on 1Pt-Cu(110)/H₂O surface. See Fig.S2 for color coding.