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Electronic Supplementary Information

Addressing the uncertainty of DFT-determined hydrogenation mechanisms over coinage metal surfaces

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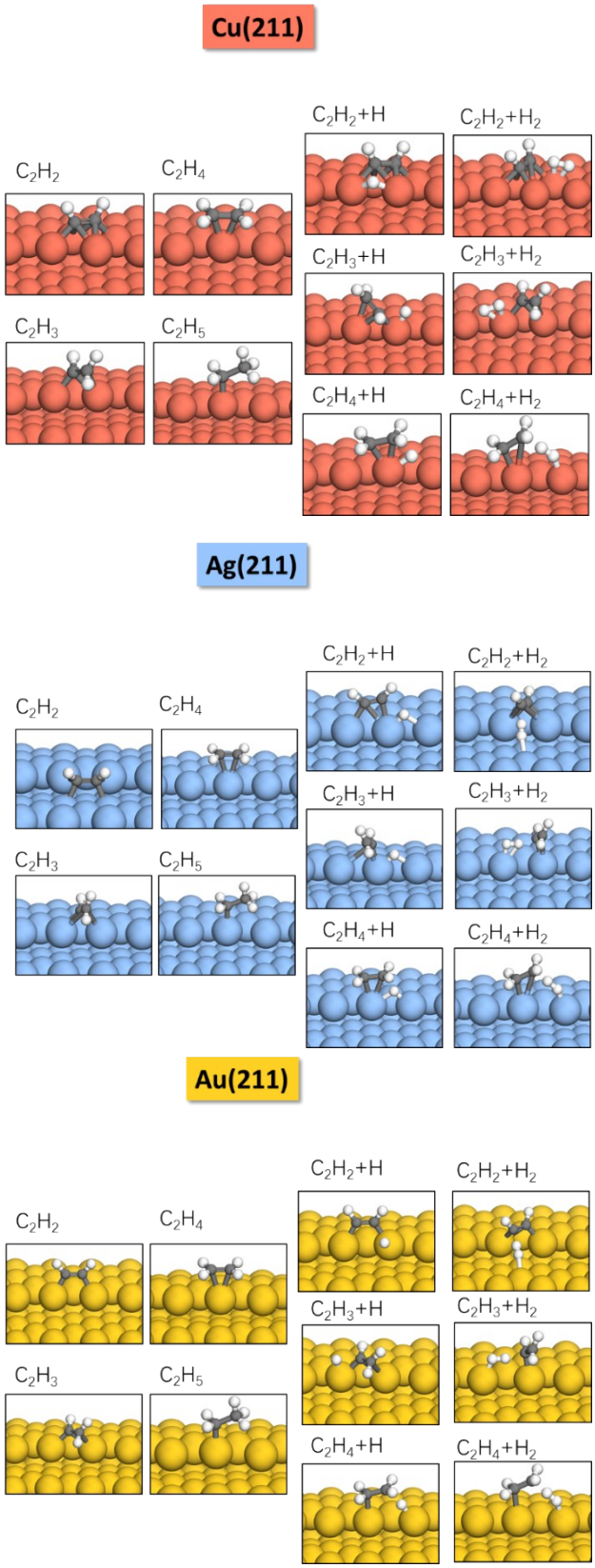


Figure S1. Optimized adsorption structures and transition state structures for the hydrogenation of C_2H_2, C_2H_3 and C_2H_4 over Cu(211), Ag(211) and Au(211). The red,

blue, yellow, grey and white balls denote the copper, silver, gold, carbon and hydrogen atoms, respectively. This notation is used throughout this paper.

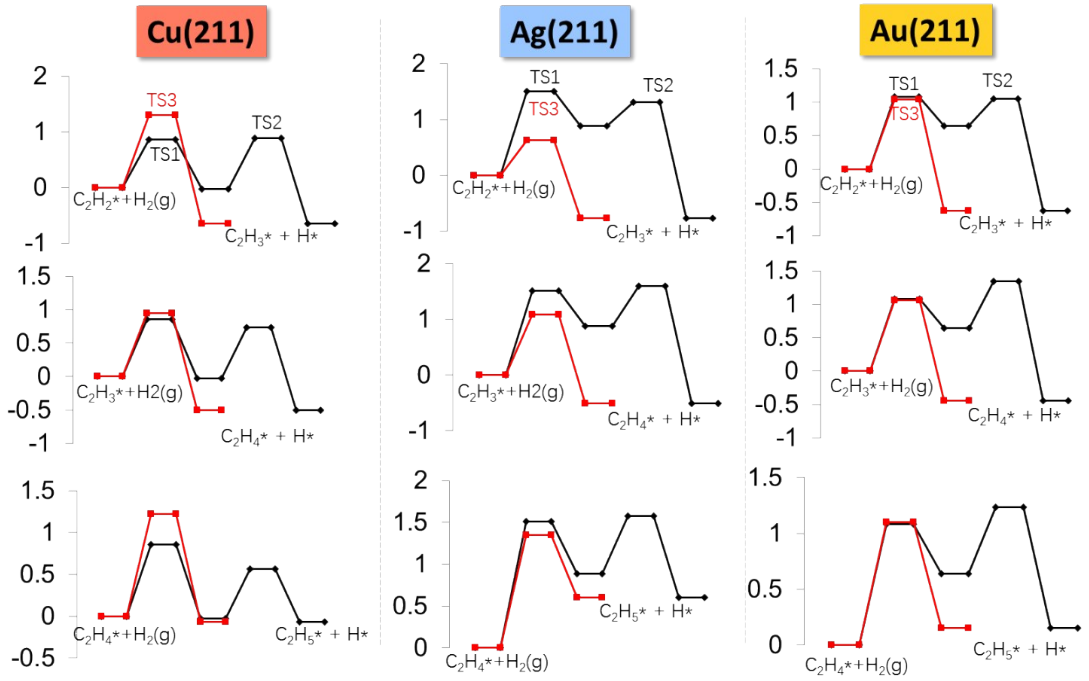
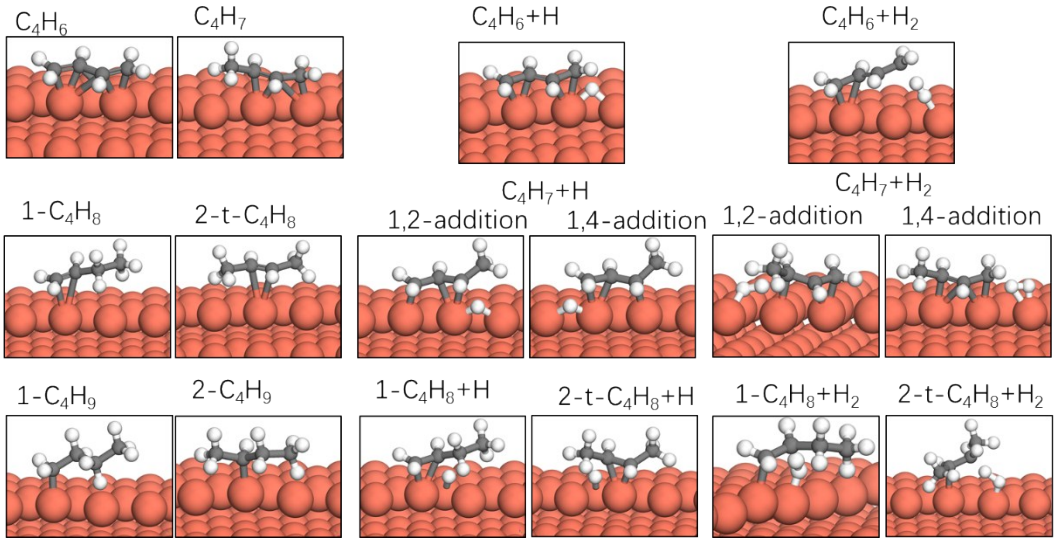
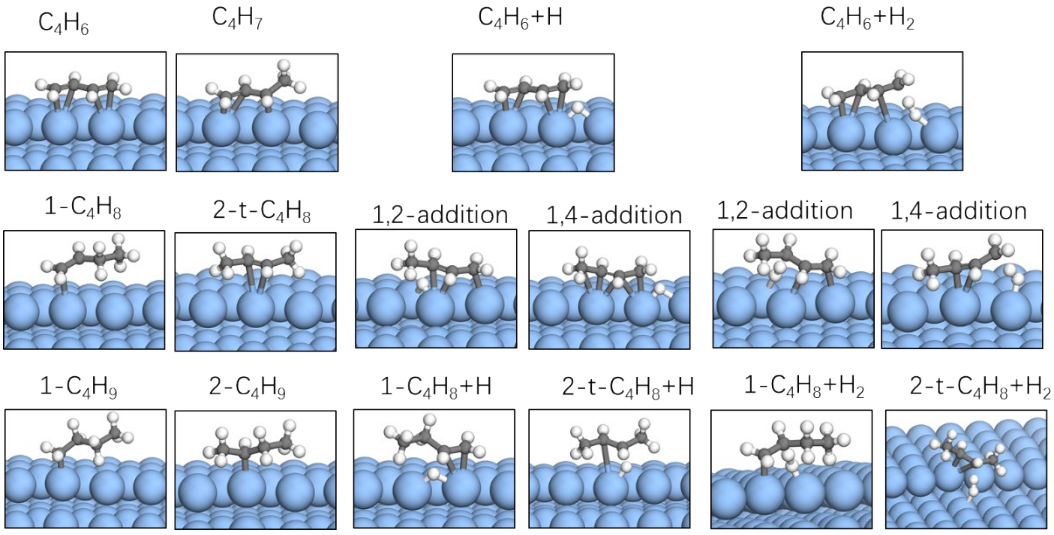


Figure S2. Energy profiles of C_2H_2, C_2H_3 and C_2H_4 hydrogenation over Cu(211), Ag(211) and Au(211). The black and red line represents the pathway following the HP and non-HP mechanism, respectively. This color code is used throughout this work. The transition states in HP mechanism are denoted as TS1 and TS2, respectively.

Cu(211)


C_4H_6
C_4H_7
C_4H_6+H
C_4H_6+H_2
1-C_4H_8
2-t-C_4H_8
C_4H_7+H
1,2-addition
1,4-addition
C_4H_7+H_2
1,2-addition
1,4-addition
1-C_4H_9
2-C_4H_9
1-C_4H_8+H
2-t-C_4H_8+H
1-C_4H_8+H_2
2-t-C_4H_8+H_2

Ag(211)


C_4H_6
C_4H_7
C_4H_6+H
C_4H_6+H_2
1-C_4H_8
2-t-C_4H_8
1,2-addition
1,4-addition
1,2-addition
1,4-addition
1-C_4H_9
2-C_4H_9
1-C_4H_8+H
2-t-C_4H_8+H
1-C_4H_8+H_2
2-t-C_4H_8+H_2

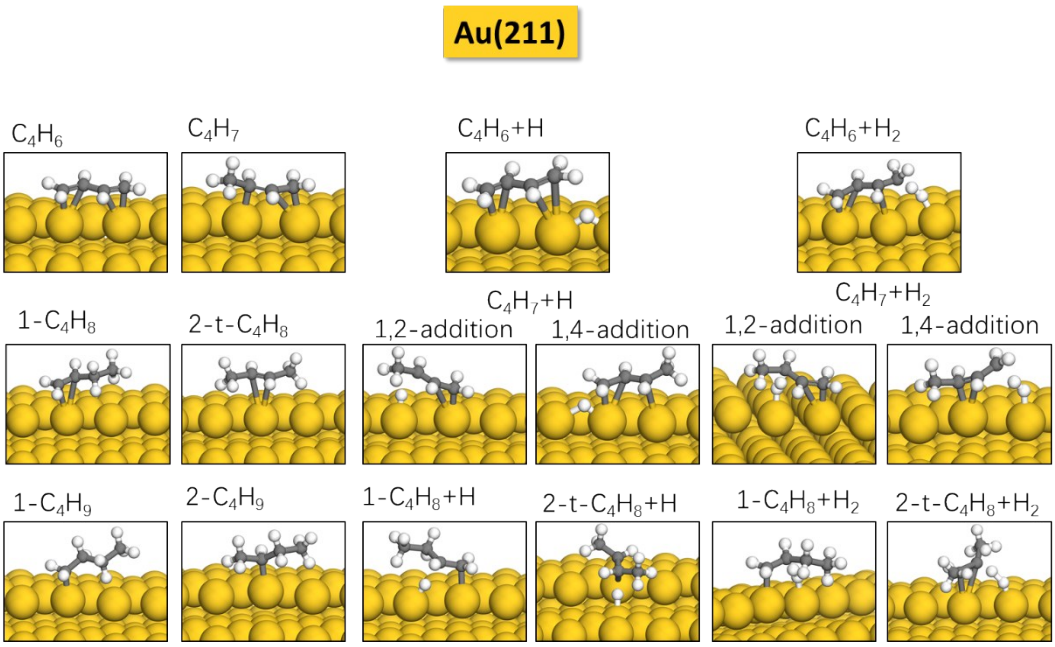


Figure S3. Optimized adsorption structures and transition state structures for the hydrogenation of C_4H_6, C_4H_7 and C_4H_8 over Cu(211), Ag(211) and Au(211).

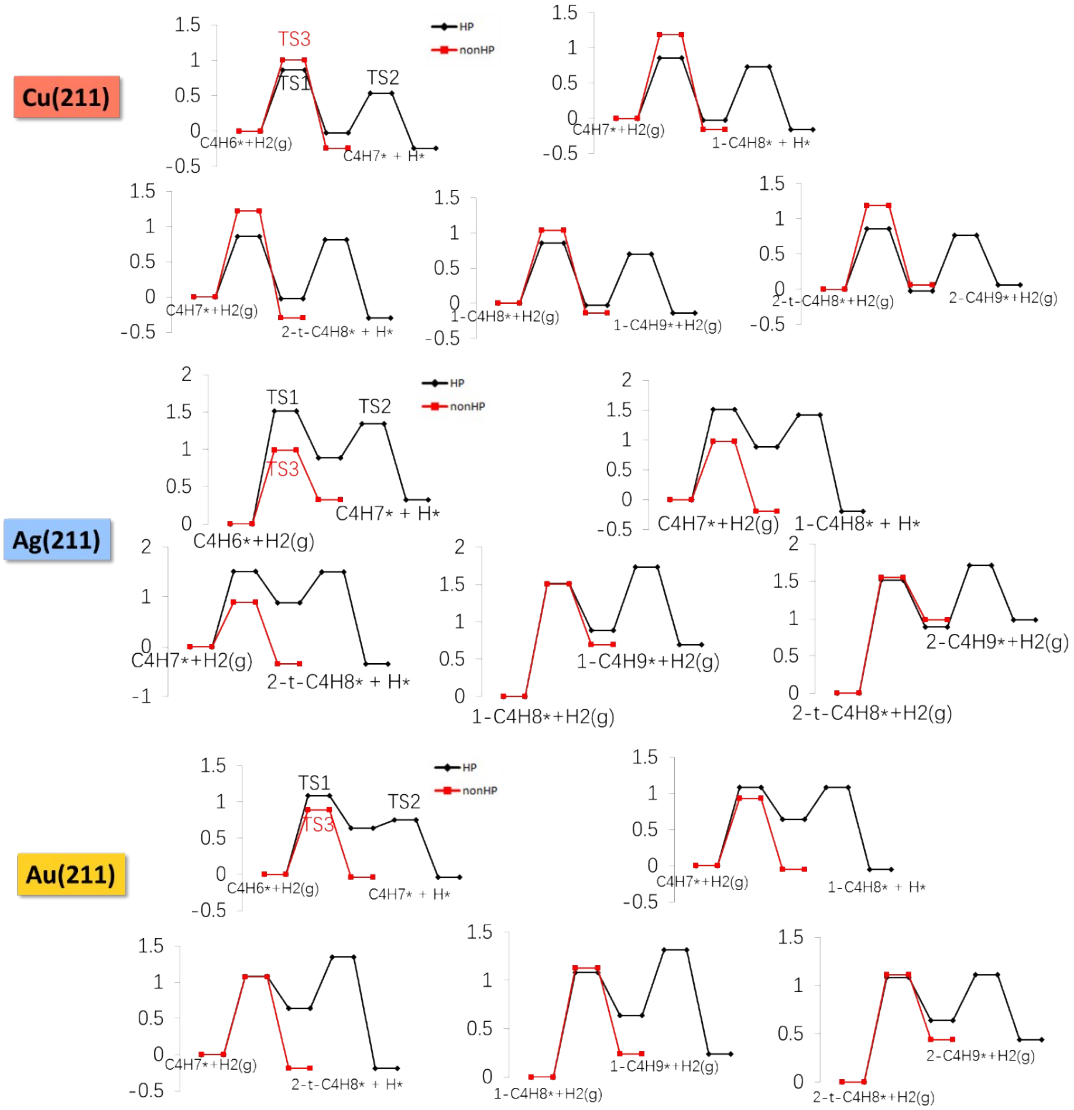


Figure S4. Energy profiles of C_4H_6, C_4H_7 and C_4H_8 hydrogenation over Cu(211), Ag(211) and Au(211).