

Supplementary Materials

Theoretical Studies of Acrolein Hydrogenation to Propenol and Propanal on Au₃ and Au₅

Guo-Jun Kang, Shuai He and Xue-Feng Ren

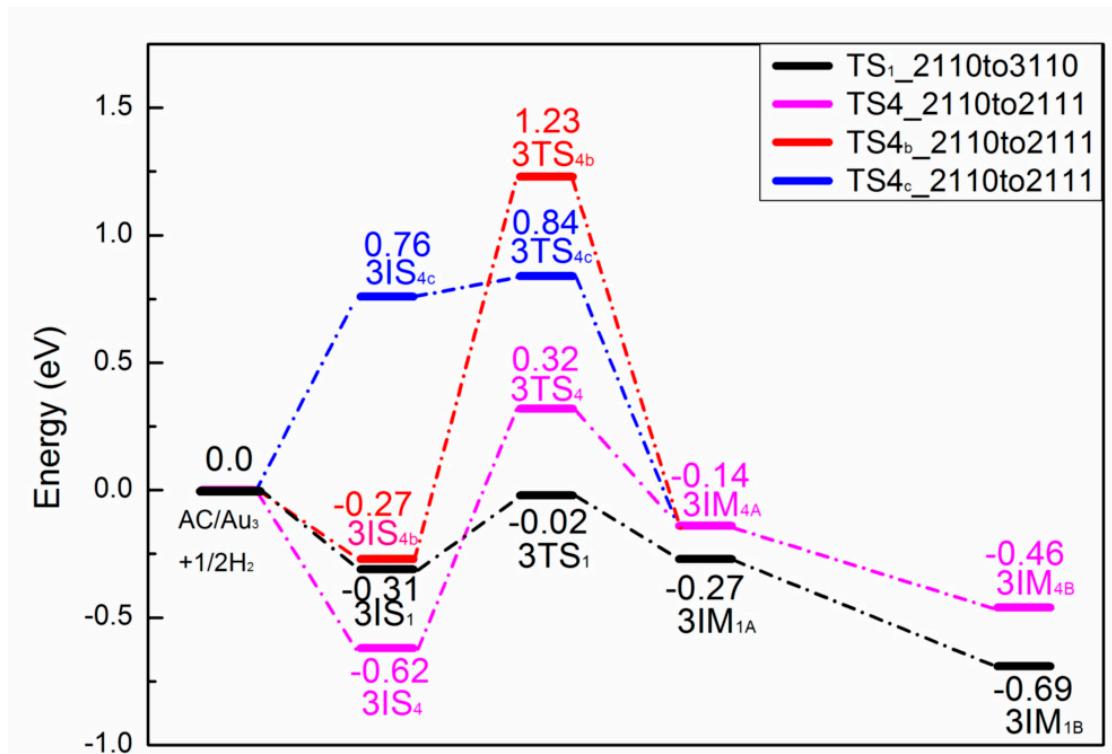


Figure A1 Potential energy surfaces of first hydrogenation step of acrolein on Au₃.

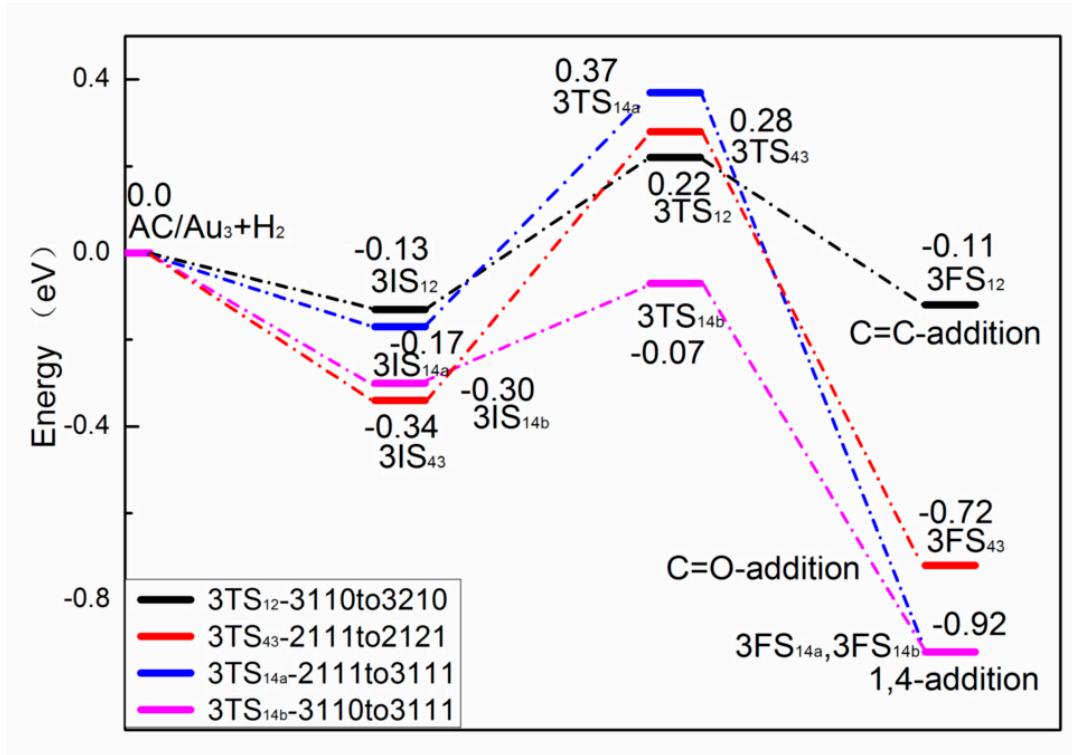


Figure A2 Potential energy surfaces of second hydrogenation step of acrolein on Au_3 .

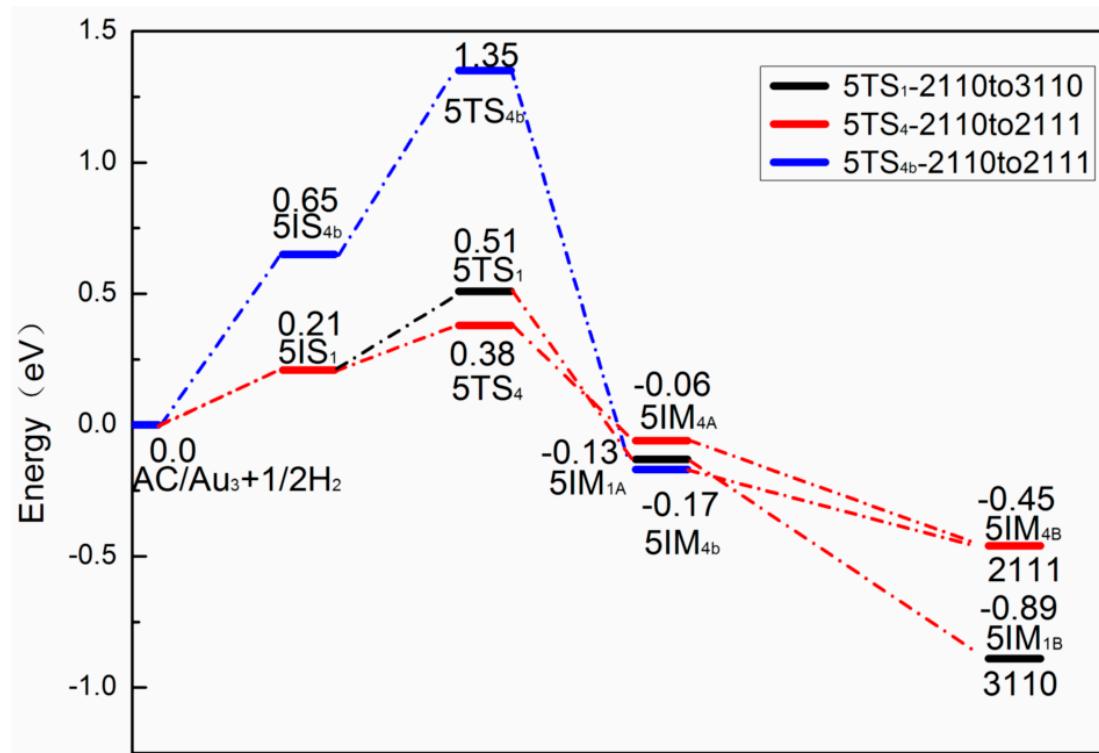


Figure A3 Potential energy surfaces of first hydrogenation step of acrolein on Au_5 .

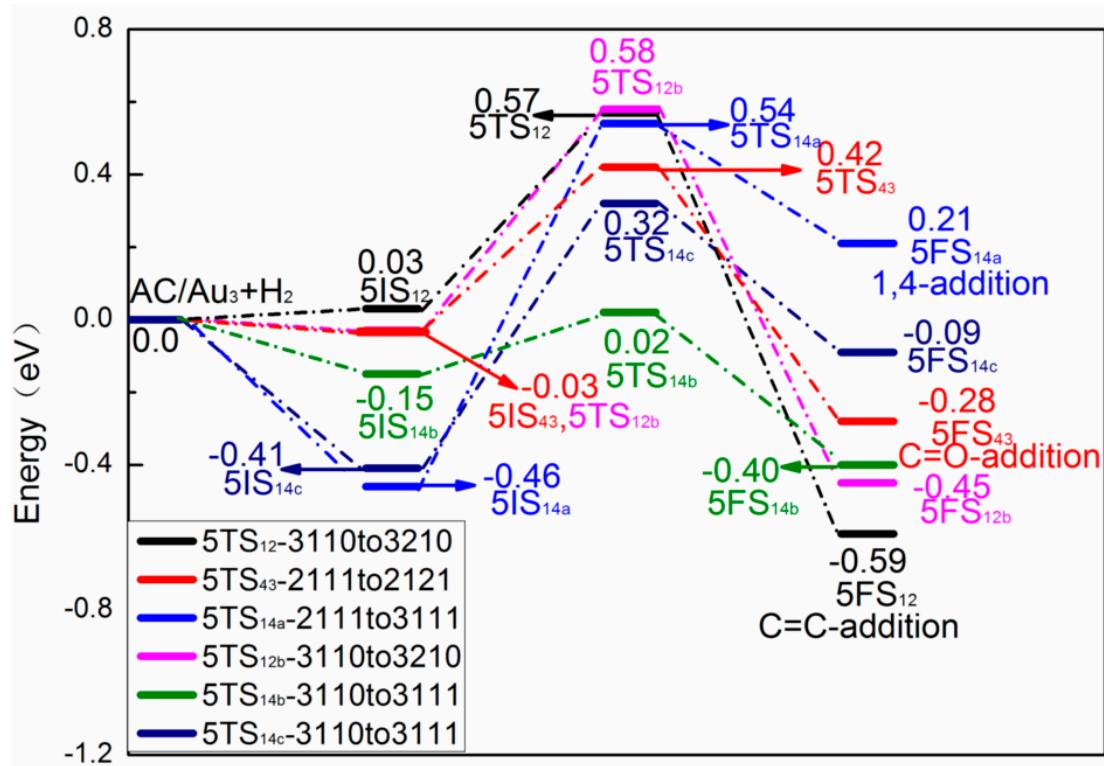


Figure A4 Potential energy surfaces of second hydrogenation step of acrolein on Au_5 .