Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

Electronic Supplementary Information (ESI)

The first principles studies on the reaction pathway of the oxidative dehydrogenation of ethane on the undoped and doped carbon catalyst

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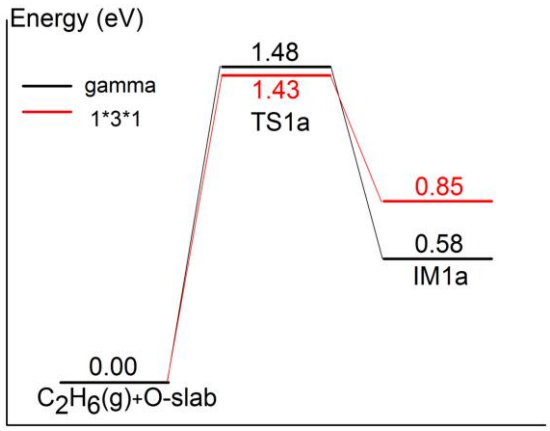

Figure S1: The part of the reaction pathway on the undoped diketone group at the armchair termination is calculated by using gamma and 1x3x1 kpoints mesh respectively.

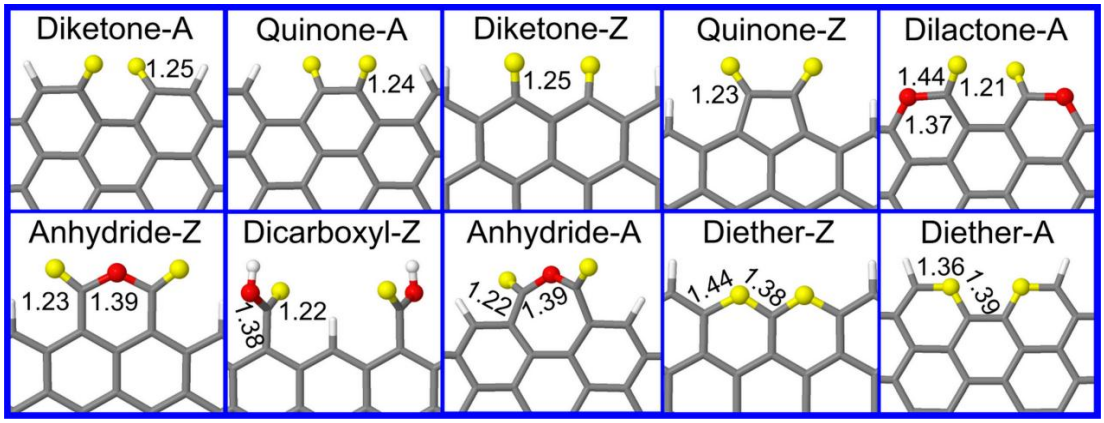

Figure S2: The optimized structures of the various oxygen functional groups and the bond distance is in Å. The yellow sites indicate the oxygens for the chemisorption of propane.

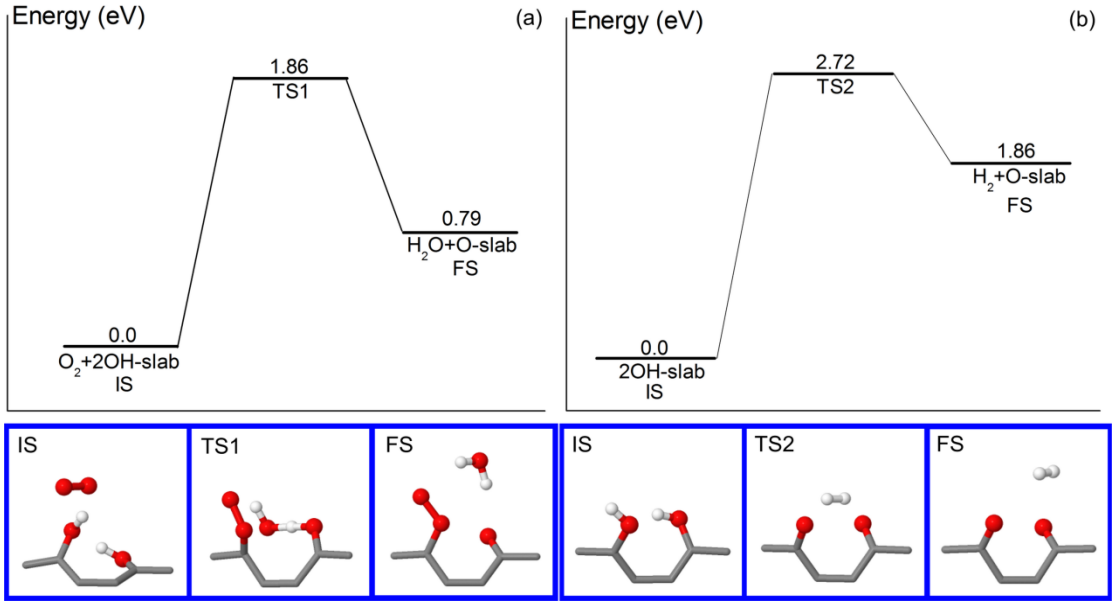

Figure S3: The energy profile of the reoxidation of the diketone sites and the related structures on the reaction pathway. Color code: carbon on the substrate is gray, carbon in ethane is violet, hydrogen is white, and oxygen is red.

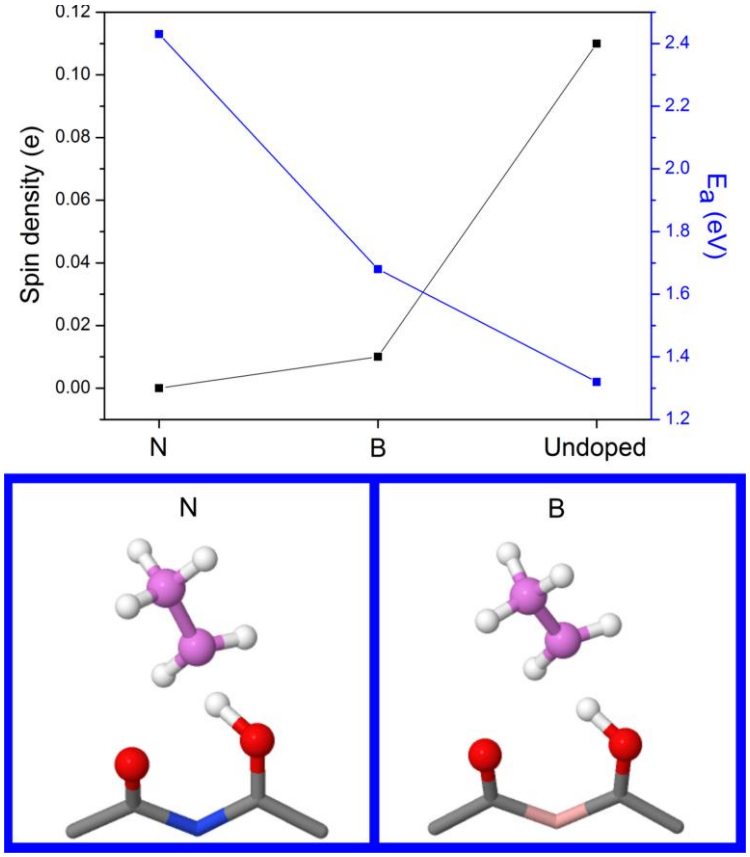

Figure S4: The relationship between the barrier (E_a) of the first C-H bond breaking in the ethane molecule and the spin density of the oxygen in diketone group at the zigzag termination which abstracts the hydrogen for the undoped, nitrogen (N), and boron (B) doping respectively.

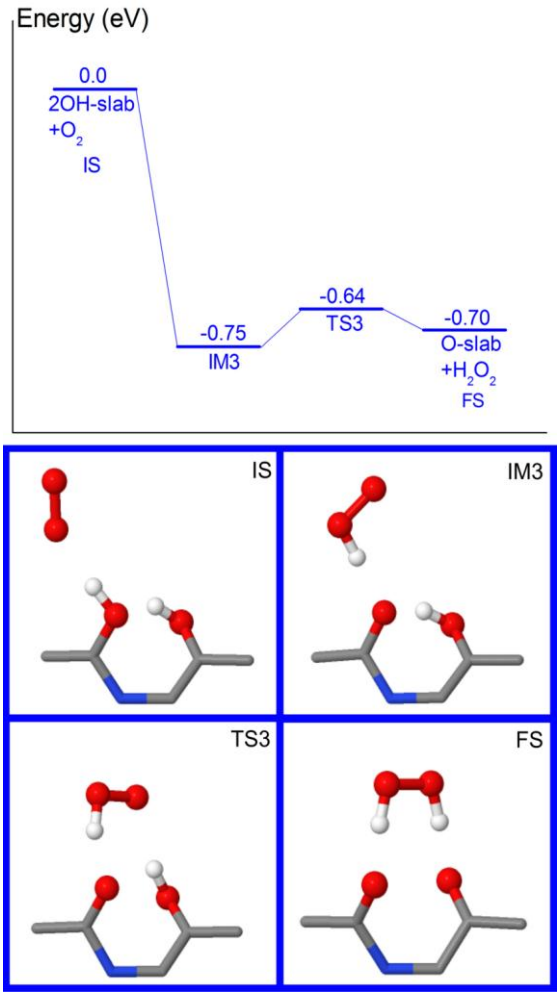

Figure S5: The energy profile of the reoxidation of the nitrogen doped diketone sites and the related structures on the reaction pathway. Color code: carbon on the substrate is gray, carbon in ethane is violet, hydrogen is white, and oxygen is red, and nitrogen is blue.

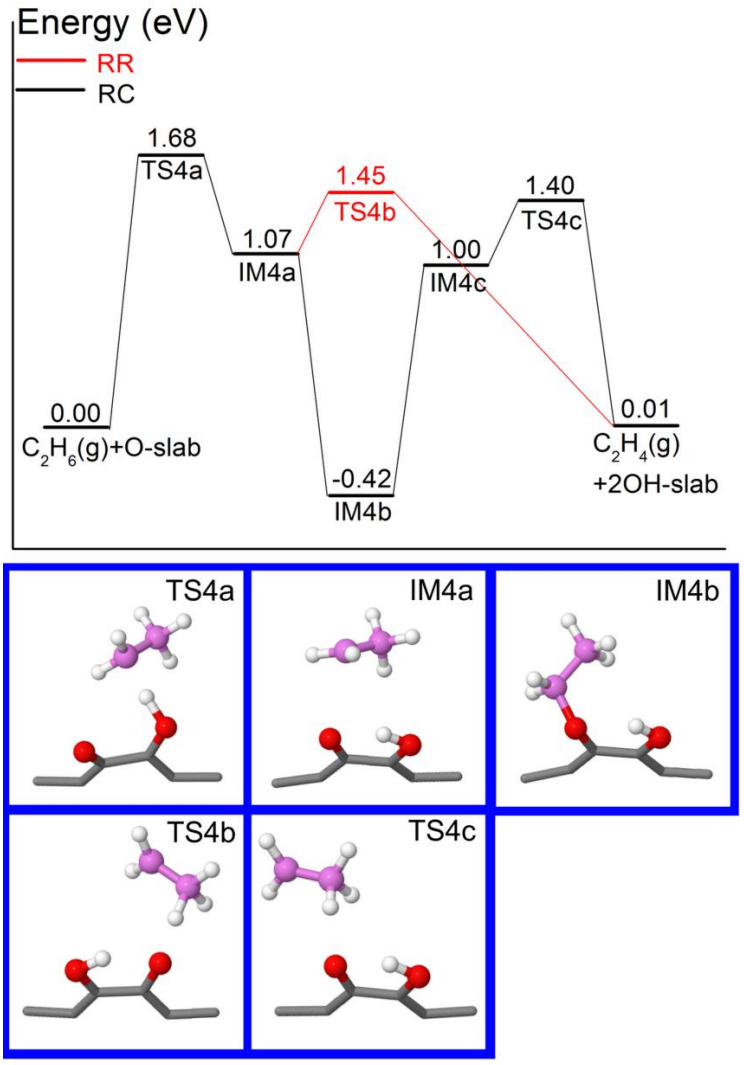

Figure S6: The energy profile of the ethane activation at the quinone site and the related structures on the reaction pathway. Color code: carbon on the substrate is gray, carbon in ethane is violet, hydrogen is white, and oxygen is red.

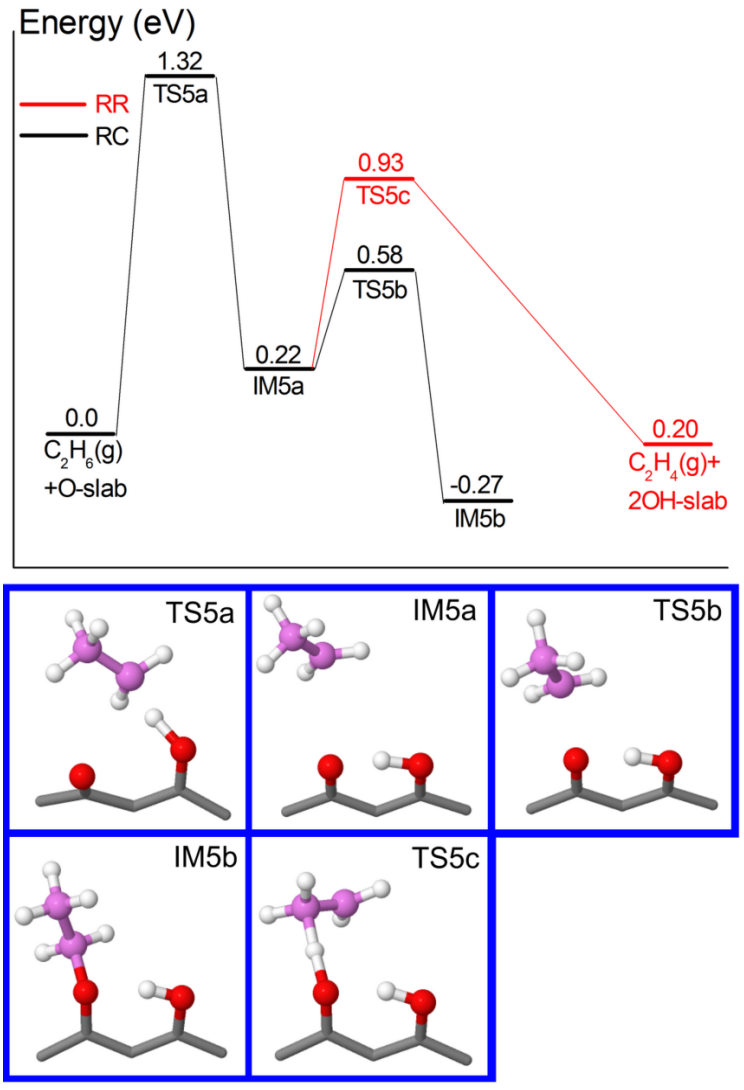

Figure S7: The energy profile of the ethane activation at the diketone site on zigzag terminated edge and the related structures on the reaction pathway. Color code: carbon on the substrate is gray, carbon in ethane is violet, hydrogen is white, and oxygen is red.