Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information

Selective Hydrogenation of 1, 3-Butadiene Catalyzed by A Single Pd Atom Anchored on Graphene: The Importance of Dynamics

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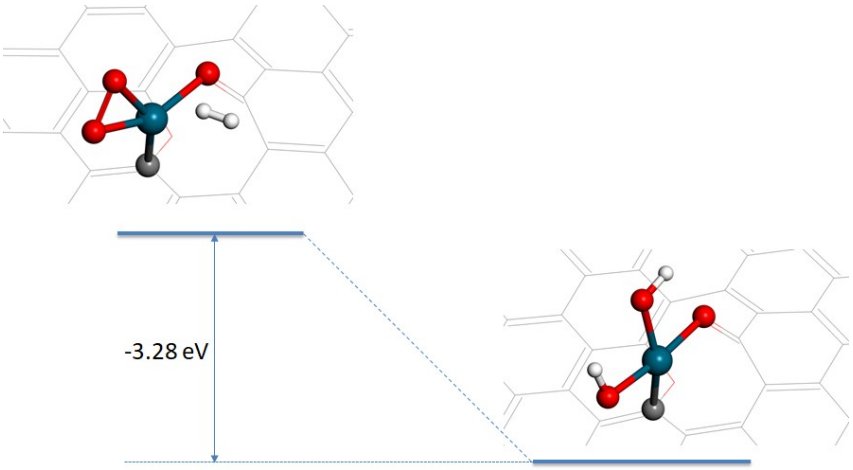

Figure S1. Energetics and geometry for the hydrogenation of the oxygen atoms on Pd.

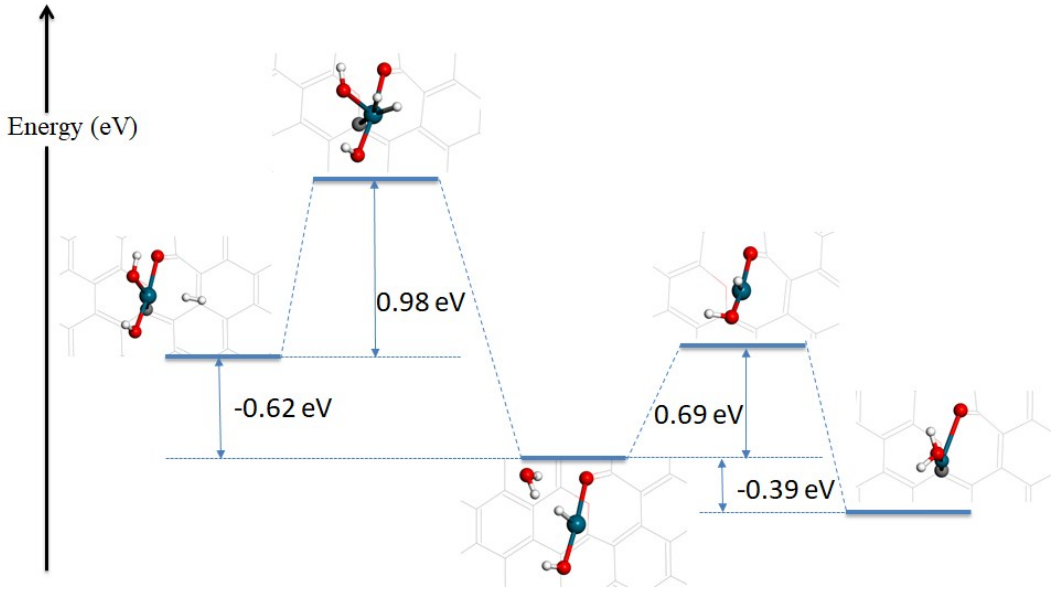

Figure S2. Energetics and geometry for the reaction of water formation on Pd.

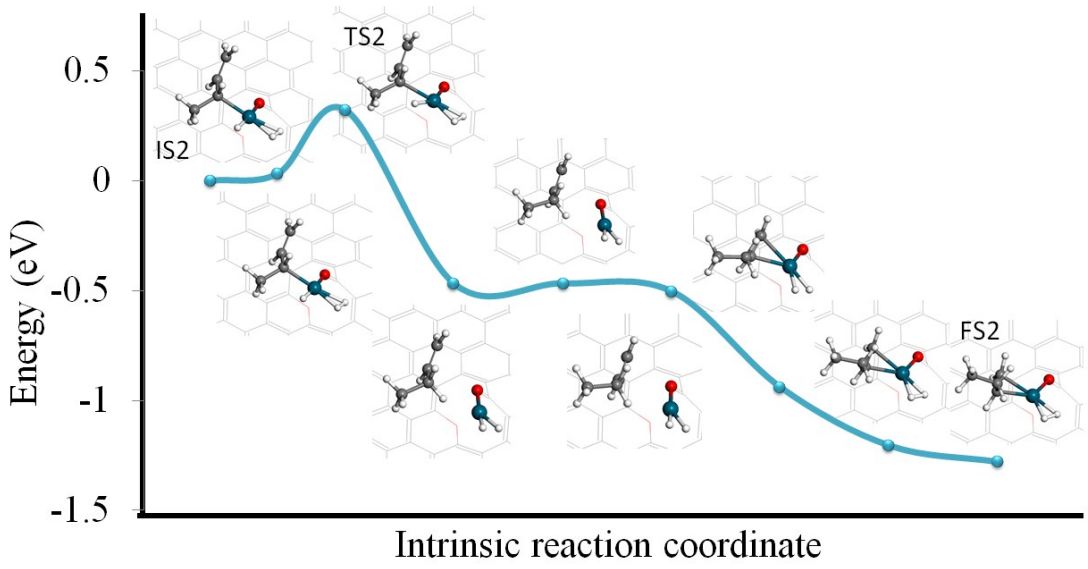

Figure S3. Minimum energy path from TS2 to 1B* obtained from NEB calculations.

Table S1 The adsorption energies for Pd, 1,3-butadiene and butane with and without Grimme' s semi-empirical scheme. From the test results, it is clear that the Grimme' s semi-empirical scheme is important for the dispersion interaction.

	E_{Pd}	$E_{1,3\text{-butadiene}}$	E_{butane}
With Grimme' s scheme	-1.87	-1.66	-0.56
Without Grimme' s scheme	-1.44	-1.30	-0.08