Insight into Mechanism and Selectivity of Propane Dehydrogenation over the Pd-Doped Cu(111) Surface

SUPPORTING INFORMATION

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Table S1. Energy barriers for propane/propylene dehydrogenation on pure and Pd-doped Cu(111) surfaces with the van der Waals correction by vdW-DF functional.

Surfaces	a	b	c	d	e
step1 (kcal/mol)	38.8	34.6	33.8	31.5	30.6
Step2 (kcal/mol)	36.9	32.9	31.4	30.5	28.7
Step3 (kcal/mol)		1.8	1.8	2.0	4.7
Step4 (kcal/mol)		2.3	2.0	1.6	3.7
Step5 (kcal/mol)		20.7	21.5	21.1	21.4
Step6 (kcal/mol)		20.6	20.8	21.1	20.7
Step7 (kcal/mol)		38.2	37.8	37.2	36.0
Step8 (kcal/mol)		38.7	38.1	37.3	36.0
Step9 (kcal/mol)		65.1	64.3	63.2	63.3