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Supporting Information

OEEFs Precisely Regulating the Propane Oxidation Reaction Catalyzed by O-Fe-Corrolazine

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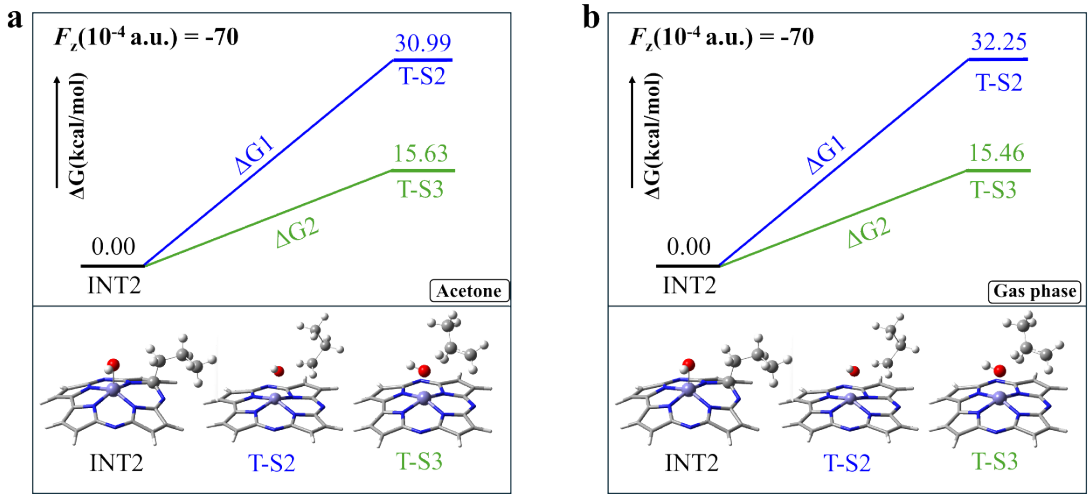

Fig. S1. The energy profile of the rate-determining steps for propane selective oxidation catalyzed by O-Fe Corrolazine with F_{z1} (10^{-4} a.u.) of -70 in gas phase and acetone solvents, which are the OH transfer step for propanol ΔG1 and the second dehydrogenation step for propylene ΔG2.

Table S1. The relative energies (kcal/mol) in gas phase and acetone solvent without OEEFs.

	Species					
	R-C	T-S1	INT1	INT2	T-S2	T-S3
Gas phase	0.00	21.34	11.06	-19.56	13.38	6.80
Acetone	0.00	22.50	11.98	-18.14	10.17	6.06

Table S2. The calculated energy barriers (kcal/mol) of propane oxidation reaction in gas phase and acetone solvent with the F_{z1} (10^{-4} a.u.) of -70.

F_{z1} (10^{-4} a.u.)		Free energy (kcal/mol)	
		acetone	gas phase
-70	ΔG1	30.99	32.55
	ΔG2	15.63	15.46