Mn Monolayer Modified Rh(100) Surface Catalyst for Syngas-to-Ethanol Conversion: A First-Principles Study

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TABLE S1. Adsorption energies of CO, C, and O on Rh(100), MnRh/Rh(100), and Mn/Rh(100) at differenct adsorbed sites. The adsorption energies of the most energy-favorable site were highlighted in bold.

	Rh(100)	MnRh/Rh(100)	Mn/Rh(100)
		CO	
top	1.78 eV	Rh: **1.95 eV** Mn: 1.11 eV	**2.38 eV**
bridge	**1.91 eV**	1.62 eV	1.38 eV
hollow	1.84eV	1.73 eV	untilt: 2.02 eV tilt: 2.31
		C	
	Rh(100)	MnRh/Rh(100)	Mn/Rh(100)
top	5.32 eV	Rh: 3.11 eV Mn: 4.49 eV	6.30 eV
bridge	6.46 eV	4.76 eV	6.51 eV
hollow	**7.80 eV**	**7.60 eV**	**8.30 eV**
		O	
	Rh(100)	MnRh/Rh(100)	Mn/Rh(100)
top	3.81 eV	Rh: 3.14 eV Mn: 1.47 eV	5.53 eV
bridge	4.03 eV	4.17 eV	6.34 eV
hollow	**4.90 eV**	**5.53 eV**	**6.70 eV**

TABLE S2. Adsorption energies (in eV) of H and CH_x (x = 1–3) at different adsorbed sites on Mn/Rh(100) and Rh(100). The adsorption energies of the most energy-favorable site were highlighted in bold.

	H		**CH**		**CH_2**		**CH_3**	
	Mn/Rh(100)	Rh(100)	Mn/Rh(100)	Rh(100)	Mn/Rh(100)	Rh(100)	Mn/Rh(100)	Rh(100)
top	2.09	2.43	6.21	4.76	4.21	3.27	2.47	**2.44**
bridge	**2.81**	2.74	6.23	6.11	4.07	4.00	**2.71**	2.43
hollow	2.73	**2.76**	**7.30**	**6.95**	**4.22**	**4.07**	2.44	2.34

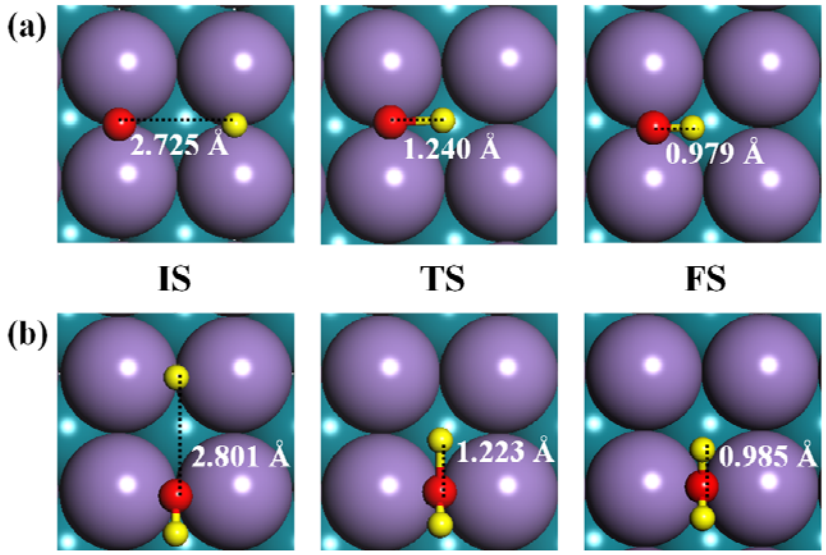

Figure S1. Atomic configurations of the initial state (**IS**), transition state (**TS**), and final state (**FS**) for OH (a) and H_2O (b) on Mn/Rh(100) surface. Color scheme: Rh, dark green; Mn, purple; O, red; H, yellow.