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Supporting information

Kinetic aspects of chain growth in Fischer-Tropsch synthesis

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Table S1: List of all elementary reaction steps surfaces and their corresponding forward and backward activation energies used to model FT synthesis over Ru(11-21). The reported forward and reverse energies are in relation to the most stable states found for the reactants and products and include zero-point-energy corrections.

Index	Elementary reaction	Forward E_{act} (kJ/mol)	Backward E_{act} (kJ/mol)
1	CO* + * → C* + O*	65	90
2	CO* + H* → HCO* + *	80	5
3	HCO* + * → CH* + O*	45	129
4	C* + H* → CH* + *	40	39
5	CH* + H* → CH_2* + *	75	37
6	CH_2* + H* → CH_3* + *	57	47
7	CH_3* + H* → CH_4 + 2*	94	57
8	C* + C* → CC* + *	138	144
9	C* + CH* → CCH* + *	129	75
10	C* + CH_2* → CCH_2* + *	*not found*	
11	C* + CH_3* → CCH_3* + *	92	116
12	CH* + CH* → CHCH* + *	149	117
13	CH* + CH_2* → $CHCH_2$* + *	*not found*	
14	CH* + CH_3* → $CHCH_3$* + *	*not found*	
15	CH_2* + CH_2* → CH_2CH_2* + *	54	60
16	CH_2* + CH_3* → CH_2CH_3* + *	*not found*	
17	CC* + H* → CCH* + H*	104	72
18	CCH* + H* → CCH_2* + *	82	129
19	CCH_2* + H* → CCH_3* + *	19	4
20	CCH* + H* → CHCH* + *	140	162
21	CCH_2* + H* → $CHCH_2$* + *	82	21

22	$CCH_3^* + H^* \rightarrow CHCH_3^* + *$	82	8
23	$CHCH^* + H^* \rightarrow CHCH_2^* + *$	83	46
24	$CHCH_2^* + H^* \rightarrow CHCH_3^* + *$	62	34
25	$CHCH_2^* + H^* \rightarrow CH_2CH_2^* + *$	45	42
26	$CHCH_3^* + H^* \rightarrow CH_2CH_3^* + *$	19	23
27	$CH_2CH_2^* + H^* \rightarrow CH_2CH_3^* + *$	58	34
28	$CH_2CH_3^* + H^* \rightarrow CH_3CH_3^* + *$	112	71
29	$O^* + H^* \rightarrow OH^* + *$	97	49
30	$OH^* + H^* \rightarrow H_2O^* + *$	89	15
31	$2OH^* \rightarrow H_2O^* + O^*$	54	11

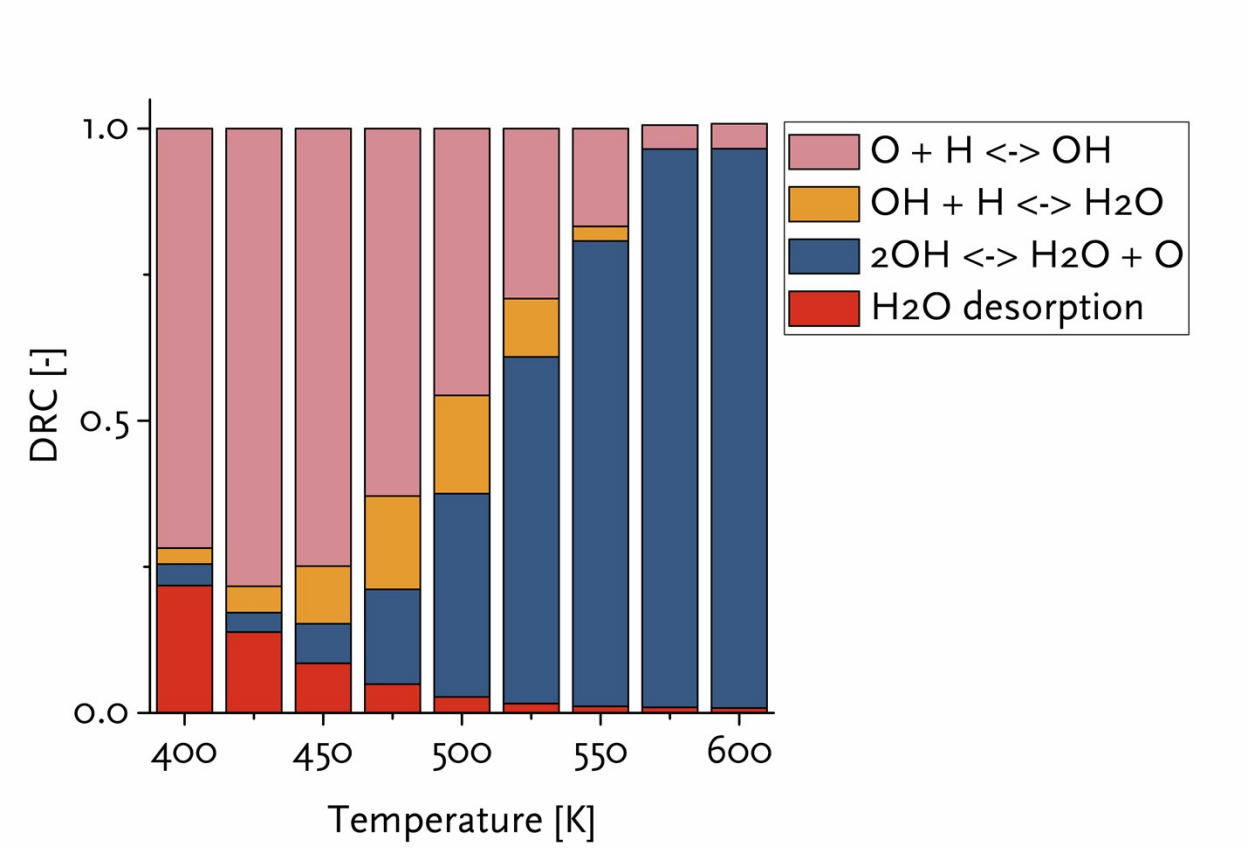

Figure S1: Degree of rate control for the microkinetics simulations of the stepped Ru surface at 20 atm and H_2/CO = 2, exemplifying that under all conditions O removal from the surface is controlling the overall CO consumption rate.