Supporting Information

Table S4. Condensed Fukui function for the zeolite cluster and molecules (in atomic units). The functions are calculated by means of finite-difference approximation, using Mulliken and Hirshfeld charges. For HF/6-31G** and DFT methods the functions are obtained with (*) ± 1·0 electron and (**) ± 0·1 electron occupations, respectively.

	Fukui function					
	HF/6-31G**		BLYP/DNP			
System	Mulliken (*)		Mulliken (**)		Hirshfeld (**)	
3T cluster-1	f^-	f^+	f^-	f^+	f^-	f^+
H_8	0·01843	0·09123	0·01900	0·27800	0·01300	0·14500
Al	0·04901	0·05690	0·11800	–0·05800	0·10200	0·06800
O_3	0·05930	–0·02807	0·12800	–0·02100	0·11400	0·01400
O_4	–0·00725	–0·12221	–0·01500	–0·13700	0·00300	0·07700
O_5	0·55819	0·00406	0·19400	0·00800	0·19200	0·02400
O_6	0·04118	–0·02216	0·10800	–0·03100	0·11100	0·00400
Si_1	–0·01859	0·79918	–0·01800	0·54600	0·02500	0·30300
Si_2	–0·03901	0·00836	–0·01200	0·03500	0·09600	0·41000
3T cluster-2						
H_8	0·00473	0·11428	0·02000	0·33600	0·01300	0·16900
Al	0·01290	0·07067	0·11500	–0·04600	0·10000	0·07800
O_3	0·01595	–0·03200	0·19900	0·00300	0·19800	0·02400
O_4	–0·00729	–0·13344	-0·01900	–0·14500	0·00200	0·07700
O_5	0·03820	0·00012	0·06900	–0·02600	0·05700	0·02000
O_6	0·23703	–0·01375	0·13500	–0·02300	0·13900	0·00400
Si_1	–0·01675	0·78986	-0·01600	0·48500	0·02400	0·27500
Si_2	–0·07313	0·00642	-0·00400	0·02400	0·11400	0·03700
CH_4						
C	0·00010	–0·54451	0·17700	–0·50300	0·30800	0·23400
H	0·24998	0·38613	0·20600	0·37600	0·17300	0·19200
CO						
C	0·666609	0·755268	0·71900	0·75100	0·69700	0·66700
O	0·333391	0·244732	0·28100	0·24900	0·30300	0·33300
NH_3						
N	0·529348	–0·40705	0·55900	–0·31700	0·52500	0·25300
H	0·156904	0·469032	0·14700	0·43900	0·15800	0·24900

Table S5. Global reactivity descriptors for the zeolite cluster and molecules (in atomic units). The quantities are evaluated by the HF/6-31G**//BLYP/DNP prescription employing Koopmans' theorem.

System	Chemical potential	Global softness	Global electrophilicity
3T cluster-1	–0·16415	1·88729	0·05085
3T cluster-1	–0·16191	1·88441	0·04940
CH_4	–0·14439	1·23799	0·02581
CO	–0·19661	1·41808	0·05482
NH_3	–0·10203	1·56482	0·01629

Table S6. Condensed Fukui function, local softness and local philicity values for the zeolite cluster and molecules (in atomic units). The quantities are calculated by Koopmans' theorem using the values from the table 2. Fukui function is from DFT calculation at BLYP/DNP level of theory and Hirshfeld scheme of charge.

System	Fukui function	Local softness	Local philicity
3T cluster-1	f^+	s^+	w^+
H_8	0·11610	0·21911	0·00590
Al	0·10000	0·18873	0·00509
O_3	0·02320	0·04379	0·00118
O_4	0·05450	0·10286	0·00277
O_5	0·03640	0·06870	0·00185
O_6	0·01420	0·02680	0·00072
Si_1	0·21570	0·40709	0·01097
Si_2	0·09770	0·18439	0·00497
3T cluster-2	f^+	s^+	w^+
H_8	0·12610	0·23762	0·00623
Al	0·10630	0·20031	0·00525
O_3	0·03610	0·06803	0·00178
O_4	0·05380	0·10138	0·00266
O_5	0·02500	0·04711	0·00123
O_6	0·01520	0·02864	0·00075
Si_1	0·20620	0·38857	0·01019
Si_2	0·09090	0·17129	0·00449
CH_4			
	f^-	s^-	w^-
C	0·32440	0·40160	0·00837
H	0·16890	0·20910	0·00436
CO	f^-	s^-	w^-
C	0·66800	0·94728	0·03662
O	0·33200	0·47080	0·01820
NH_3	f^-	s^-	w^-
N	0·53860	0·84281	0·00877
H	0·15380	0·24067	0·00251