Supporting Information

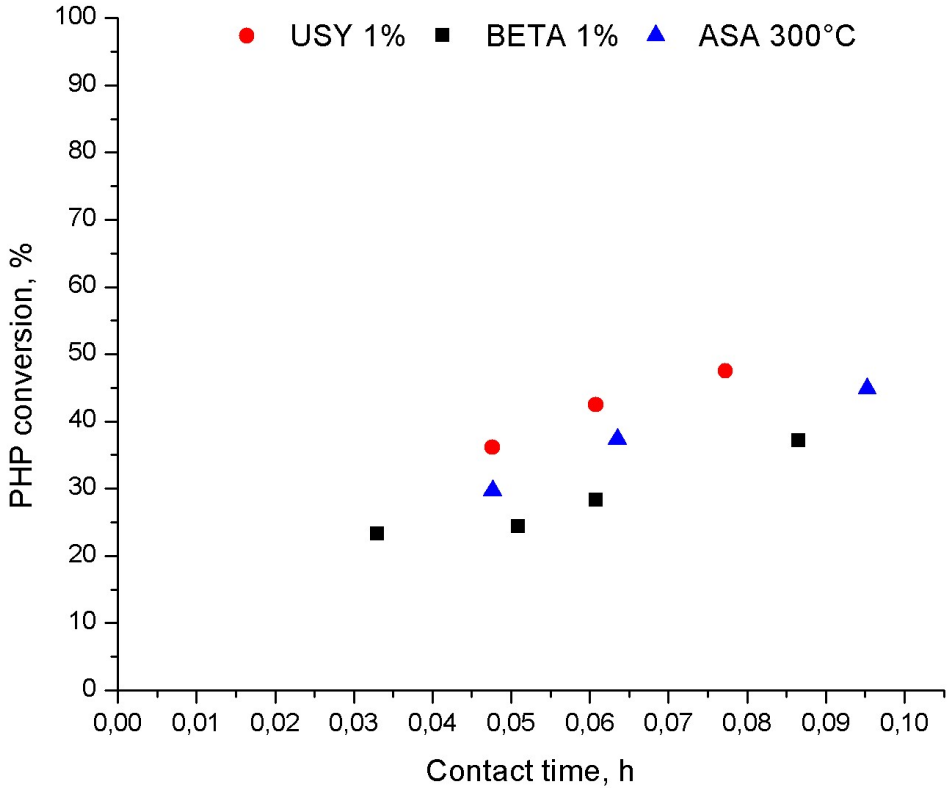

Figure S 1. Evolution of perhydrophenanthrene conversion with contact time on Pt/USY, Pt/BETA catalysts with 1 wt.% zeolite in alumina binder at 280°C; and Pt/ASA (at 300°C) bifunctional catalysts.

Models used in GCMC simulations:

Since both structures (*BEA and FAU) are assimilated to be purely siliceous, the energetic description of the system is only based on the summation of two different contributions:

$$U_{TOT} = U_{LJ} + U_{intra}$$

where the term corresponding to the dispersion-repulsion energy is described *via* a Lennard-Jones potential:

$$U_{LJ}^{ij}(r) = 4\,\varepsilon\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]$$

A collection of intramolecular terms allow accounting for the energetic contribution associated to the internal deformation/flexibility of the hydrocarbons:

$$U_{intra} = U_{bonding} + U_{bending} + U_{torsion} =$$

$$= \sum_{i=1}^{n_{bonds}} \frac{1}{2} k_b^i (d - d_0)^2 + \sum_{i=1}^{n_{angles}} \frac{1}{2} k_a^i (cos\,\theta - cos\,\theta_0)^2 + \sum_{i=1}^{n_{dihedral\ angles}} \sum_{j=1}^{8} A_i^j (cos\chi)^j$$

The different parameters used in the calculations are compiled in the following tables:

Table S1: Lennard-Jones parameters

Force center	$\sigma^{\dagger}$ [Å]	$\varepsilon^{\dagger}$ [K]	$\delta^{\dagger\dagger}$ [Å]
CH_3-AUA	3.6072	120.15	0.21584
CH_2-aliph-AUA	3.4612	86.291	0.38405
CH-aliph-AUA	3.3625	50.98	0.64599
C-cyc-AUA‡	2.440	15.035	----
CH-cyc-AUA‡	3.3625	50.98	0.64599
CH2-cyc-AUA	3.461	90.09	0.336
O-zeolite	3.00	112.236	----
Si-zeolite	0.00	0.00	----

†Lorentz-Berthelot mixing rules were employed to determine the interactions between different force center types.

††δ is the anisotropic distance used in the AUA (**A**nisotropic **U**nited **A**toms) potential.

‡ borrowed from their aliphatic counterparts

Table S2: Parameters of the harmonic bonding potential

Bond	k_b [K] †	d_0 [Å]
CH_3-AUA ---- CH_2-aliph-AUA	----	1.535
CH_2-aliph-AUA ---- CH_2-aliph-AUA	----	1.535
CH_2-aliph-AUA ---- CH-aliph-AUA	----	1.535
CH2-cyc-AUA ---- CH2-cyc-AUA	----	1.53519
CH3-AUA ---- CH2-cyc-AUA	----	1.53519
CH3-AUA ---- CH-cyc-AUA	----	1.53519
CH3-AUA ---- C-cyc-AUA	----	1.53519

†Bond lengths are considered constant

Table S3: Parameters of the harmonic bending potential

Angle	k_a [K]	θ_0 [deg]
CH3-AUA ---- CH2-aliph-AUA ---- CH2-aliph-AUA	74900	114.00
CH2-aliph-AUA ---- CH2-aliph-AUA ---- CH2-aliph-AUA	74900	114.00
CH2-cyc-AUA ---- CH2-cyc-AUA ---- CH2-cyc-AUA	74900	114.00
CH2-cyc-AUA ---- CH2-cyc-AUA ---- CH-cyc-AUA	74900	114.00
CH2-cyc-AUA ---- CH-cyc-AUA ---- CH2-cyc-AUA	74900	114.00
CH2-cyc-AUA ---- CH-cyc-AUA ---- CH-cyc-AUA	74900	114.00 (105.00)†
CH-cyc-AUA ---- CH2-cyc-AUA ---- CH-cyc-AUA	74900	114.00 (105.00)†
CH-cyc-AUA ---- CH-cyc-AUA ---- CH-cyc-AUA	74900	114.00
C-cyc-AUA ---- CH2-cyc-AUA ---- C-cyc-AUA	74900	114.00
CH2-cyc-AUA ---- CH-cyc-AUA ---- CH2-cyc-AUA	74900	114.00 (105.00)†
CH2-cyc-AUA ---- C-cyc-AUA ---- CH3-AUA	74900	114.00

†When 5-membered rings are involved

Table S4: Parameters of the torsion potential

Dihedral angle	Angle	A^0	A^1	A^2	A^3	A^4	A^5	A^6	A^7	A^8
(*) – CH2-aliph-AUA – CH2-aliph-AUA -- (*)	0	1001.36	2129.52	-303.06	-3612.27	2226.71	1965.93	-4489.34	-1736.22	2817.37
(*) – CH2-cyc-AUA – CH2-cyc-AUA -- (*)	0	1001.36	2129.52	-303.06	-3612.27	2226.71	1965.93	-4489.34	-1736.22	2817.37
(*) – CH2-cyc-AUA – CH-cyc-AUA -- (*)	0	1001.36	2129.52	-303.06	-3612.27	2226.71	1965.93	-4489.34	-1736.22	2817.37
(*) – CH-cyc-AUA – CH-cyc-AUA -- (*)	0	1001.36	2129.52	-303.06	-3612.27	2226.71	1965.93	-4489.34	-1736.22	2817.37
(*) – CH2-cyc-AUA – C-cyc-AUA -- (*)	0	1001.36	2129.52	-303.06	-3612.27	2226.71	1965.93	-4489.34	-1736.22	2817.37