

Supplementary information

Melanin Polymerization Held in Check: A Composite of Dihydroxyphenylalanine with Zeolite Beta

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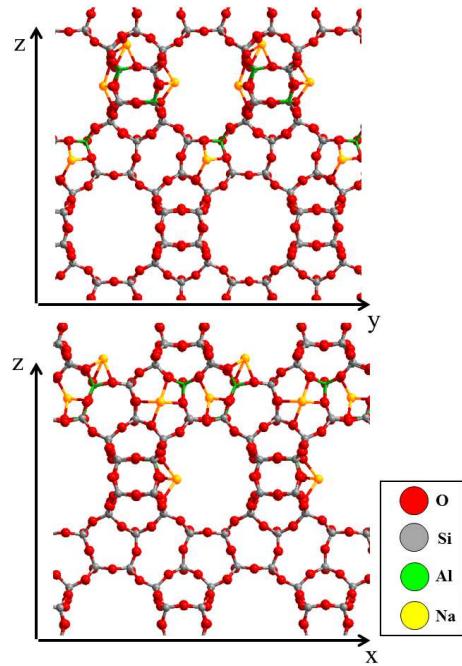


Figure SI-1. $2 \times 2 \times 1$ supercell view along the xy and yz planes of BEA-type framework showing the framework Al atoms and charge compensating Na^+ cations.

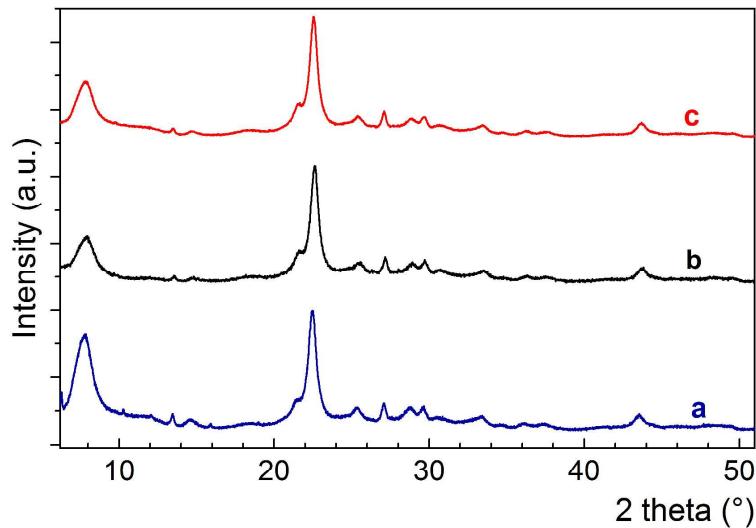


Figure SI-2. X-Ray diffraction patterns of parent zeolite Beta (a), DOPA/Beta pH nat (b) and DOPA/Beta pH 3 (c) composites.

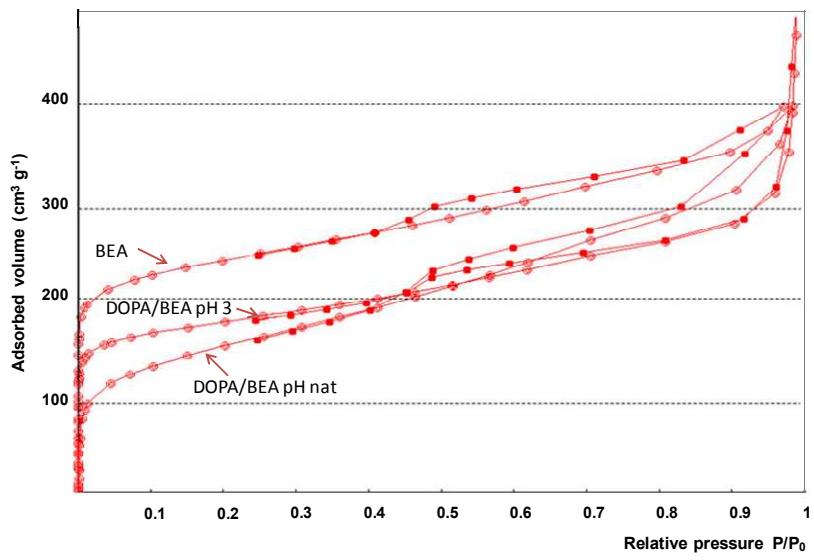


Figure SI-3. N₂ adsorption-desorption isotherms at 77K of pristine and DOPA-loaded Beta zeolites.

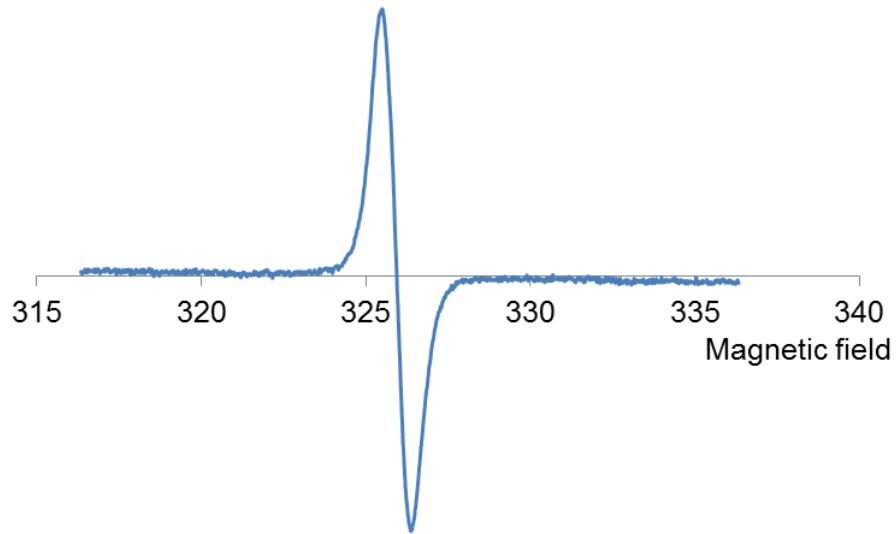


Figure SI-4. EPR spectrum of DOPA/Beta pH nat sample. Spectrum were recorded on a JEOL FA-300 series EPR spectrometer at ~9.3 GHz (X band) at 77 K.

Table SI-1. Raman bands of L-DOPA and their assignments: ν - stretching; ϕ - deformation; τ - torsion; adj - adjacent; R - ring. Figures in square brackets are P.E.D. percentages. (Values in cm^{-1})

Raman band positions (this work)	Raman band positions (Ref. 75*)	Assignment
362	366	$\phi(\text{CCN})$ adj R [23] + $\tau(\text{CCCO})$ R [18]
403	416	$\tau(\text{HOCC})$ R [91]
459	465	$\phi(\text{CCC})$ R [49] + $\tau(\text{HOCC})$ R [22]
550	553	$\tau(\text{HOCC})$ adj N [44] + $\phi(\text{CCO})$ adj R [23]
588	592	$\tau(\text{HOCC})$ adj N [51]
684	690	$\tau(\text{CCCC})$ [72]
718	720	$\tau(\text{NCC=O})$ [38]
778	782	$\tau(\text{HCCO})$ R [71]
809 (+ sh.)	809	$\tau(\text{HCCO})$ R [78]
	814	$\tau(\text{NHCH})$ [56] + $\nu(\text{CC})$ adj N [14]
838	845	$\tau(\text{HCCO})$ [78]
866	870	$\tau(\text{HCCC})$ adj R [28] + $\tau(\text{NHCH})$ [21]
919	922	$\nu(\text{CC})$ adj R [57] + $\phi(\text{CCC})$ R [14]
944	-	?
982	986	$\nu(\text{CC})$ adj N [57]
1062	1065	$\nu(\text{NC})$ [50] + $\phi(\text{HNC})$ [13] + $\phi(\text{HCN})$ [10]

1120	1124	ϕ (HCC) R [36] + ν (CCR) [17] + ϕ (HOC) R [10]
1159	1165	ϕ (HCC) R [28] + ϕ (HOC) adj N [17] + ν (CC) adj O [12]
1295	1285 (S)	τ (HCCC) adj R [54]
	1300	ϕ (HOC) adj N [28] + ν (CC) adj O [17] + ϕ (HCN) [12]
1346	1350	ν (CC) R [36] + ϕ (HOC) R [31]
1404	1407	ν (CC) R [52] + ϕ (HCC) R [16]
1438	1445	ϕ (HCH) [88]
1497	1500	ν (CC) R [53] + ϕ (HCC) adj N [16]
1610	1610	ν (C=C) R [68]
1631	-	?

* Siddiqui, S. A.; Pandey, A. K.; Dwivedi, A.; Jain, S.; Misra, N. Comparative Conformational, Structural and Vibrational Study on the Molecular Structure of Tyrosine and L-Dopa Using Density Functional Theory. *J. Chem. Pharm. Res.* **2010**, 2, 835-850.