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## **Supporting information**

## From zeolite nets to *sp*<sup>3</sup> carbon allotropes: a topology-based multiscale theoretical study

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Bond lengths and angles Elastic constants Electronic band structures Phonon dispersion curves

Structure	Bond lengths, Å	Bond angles, degrees	Shortest non-bonding distance, Å
oP24-I	1.50-1.62	94.0-123.3	2.25
oP24-II	1.51-1.59	96.2-123.0	2.28
oP28	1.49–1.59	95.5-127.8	2.27
oP20	1.52–1.62	99.1-118.0	2.31
mS32	1.51-1.65	95.0-125.9	2.27
<i>mP</i> 16	1.50-1.62	95.1-125.7	2.27

## Table S2. Elastic constants (all the values are in GPa)

## oP24-I:

	1114.561	130.016 1032.851	37.145 109.815 1132.875	0.000 0.000 0.000 525.522	0.000 0.000 0.000 0.000 434.915	$\begin{array}{c} 0.000\\ 0.000\\ 0.000\\ 0.000\\ 0.000\\ 457.698\end{array}$	
oP28	3:						
	1005.509	99.894 1124.233	164.024 53.443 1026.088	0.000 0.000 0.000 429.166	0.000 0.000 0.000 0.000 455.155	$\begin{array}{c} 0.000\\ 0.000\\ 0.000\\ 0.000\\ 0.000\\ 521.621 \end{array}$	
oP20	):						
	1049.413	44.241 1177.507	135.998 80.359 1106.605	0.000 0.000 0.000 473.426	$\begin{array}{c} 0.000\\ 0.000\\ 0.000\\ 0.000\\ 488.106\end{array}$	$\begin{array}{c} 0.000\\ 0.000\\ 0.000\\ 0.000\\ 0.000\\ 443.864 \end{array}$	
oP24	I-II:						
	983.749	62.615 1110.170	127.344 101.589 1109.028	0.000 0.000 0.000 516.412	$\begin{array}{c} 0.000\\ 0.000\\ 0.000\\ 0.000\\ 458.515\end{array}$	$\begin{array}{c} 0.000\\ 0.000\\ 0.000\\ 0.000\\ 0.000\\ 413.551 \end{array}$	
mS32	2:						
	1079.316	41.804 1145.188	86.185 96.096 1142.356	0.000 0.000 0.000 529.953	28.872 -18.470 -14.461 0.000 449.452	0.000 0.000 -22.864 0.000 416.196	
mP1	6:						
	1146.374	99.535 1145.317	86.434 39.906 1074.964	0.000 0.000 0.000 413.562	-1.673 11.968 -14.494 0.000 444.389	$\begin{array}{c} 0.000\\ 0.000\\ 14.367\\ 0.000\\ 533.109\end{array}$	

Figure S1. Electronic band structures at zero pressure [DFT-GGA(PBE)]



oP28







oP24-II





*mP*16



Figure S2. Phonon dispersion curves at zero pressure (frequencies are given in THz)





*mS*32

