Supplementary Information for Pore Size Analysis of > 250,000 Hypothetical Zeolites

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	Measured Distance (Å)
DDR	8.000
CAS	5.160
TSC	15.371
VFI	8.589
CAN	5.254
CFI	5.264
MTW	5.256
GOO	6.550
MER	9.954
DFT	4.512
ETR	8.426
MAZ	7.618
LTF	7.601

Table S.1: Hopping distances used to calculate single component diffusivities of CH_4 in the infinite dilution limit using Transition State Theory in selected zeolites.

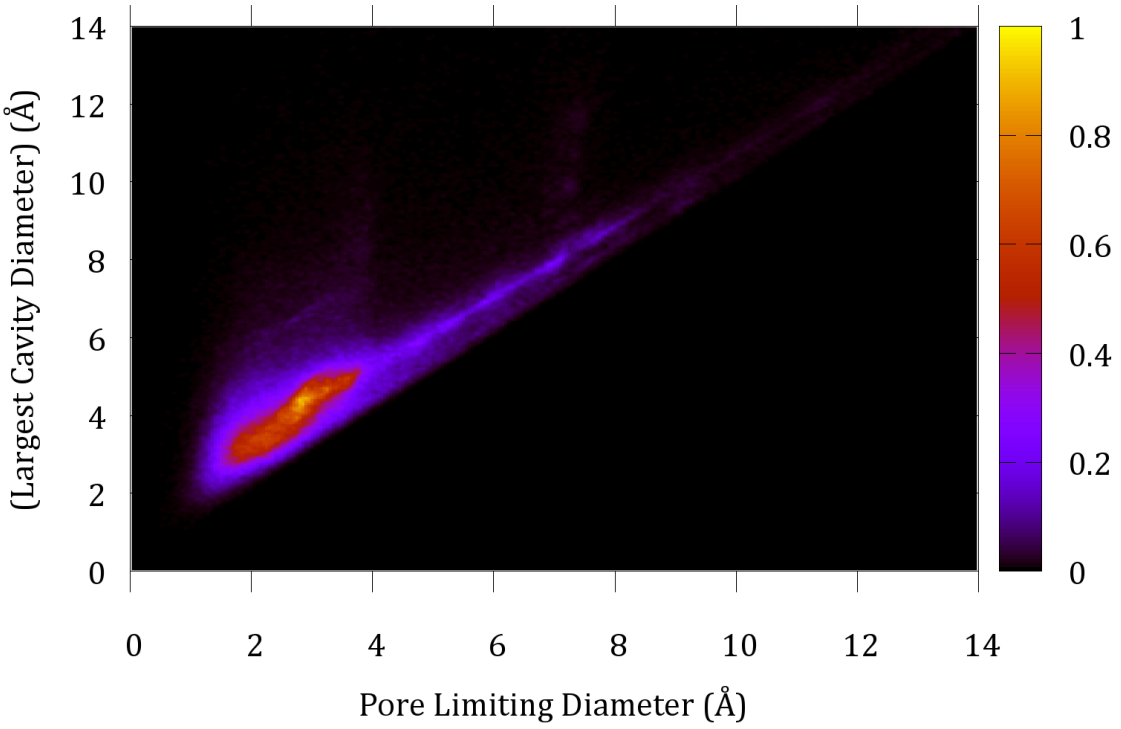

Figure S.1 The frequency of observing crystal structures with varying PLD and LCD among the full set of hypothetical zeolites. The normalization used for the color code is the same as in Figure 6.

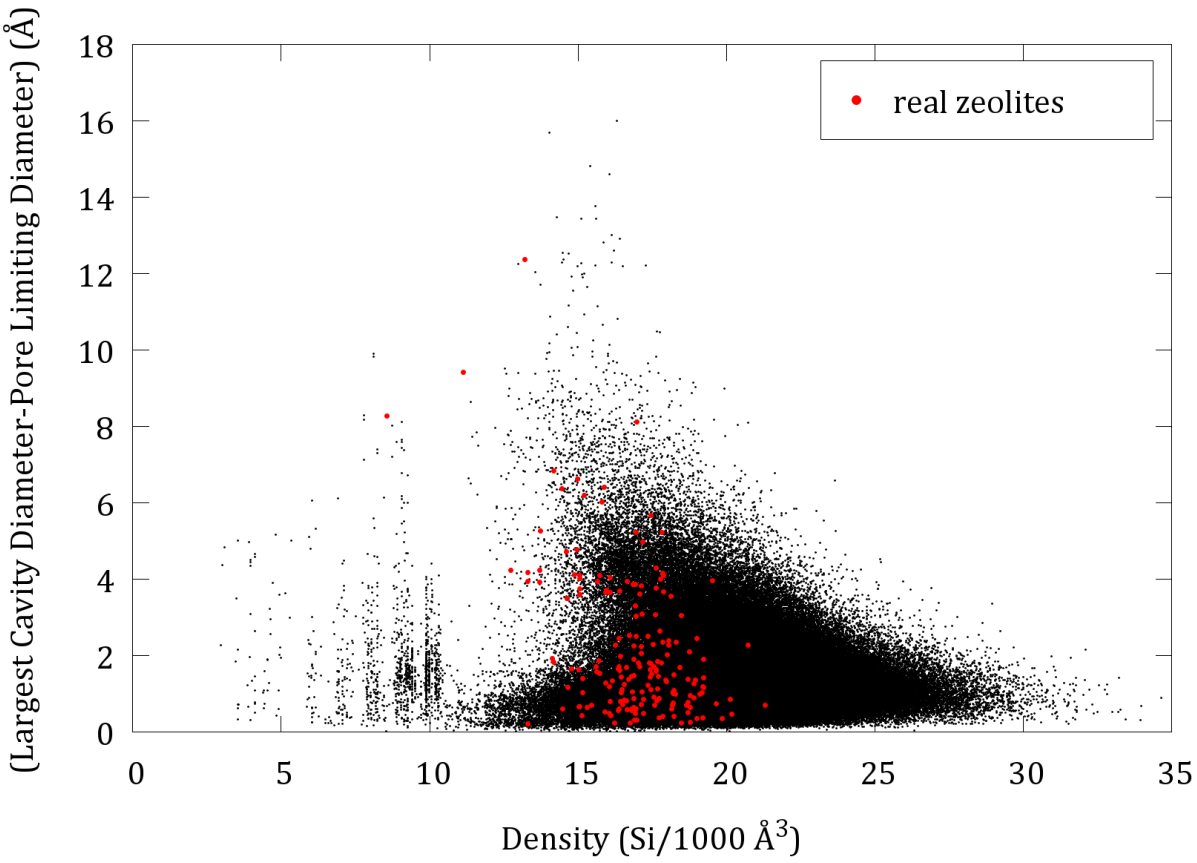

Figure S.2: The density plotted against the difference between the LCD and PLD for all the materials and the real zeolites.

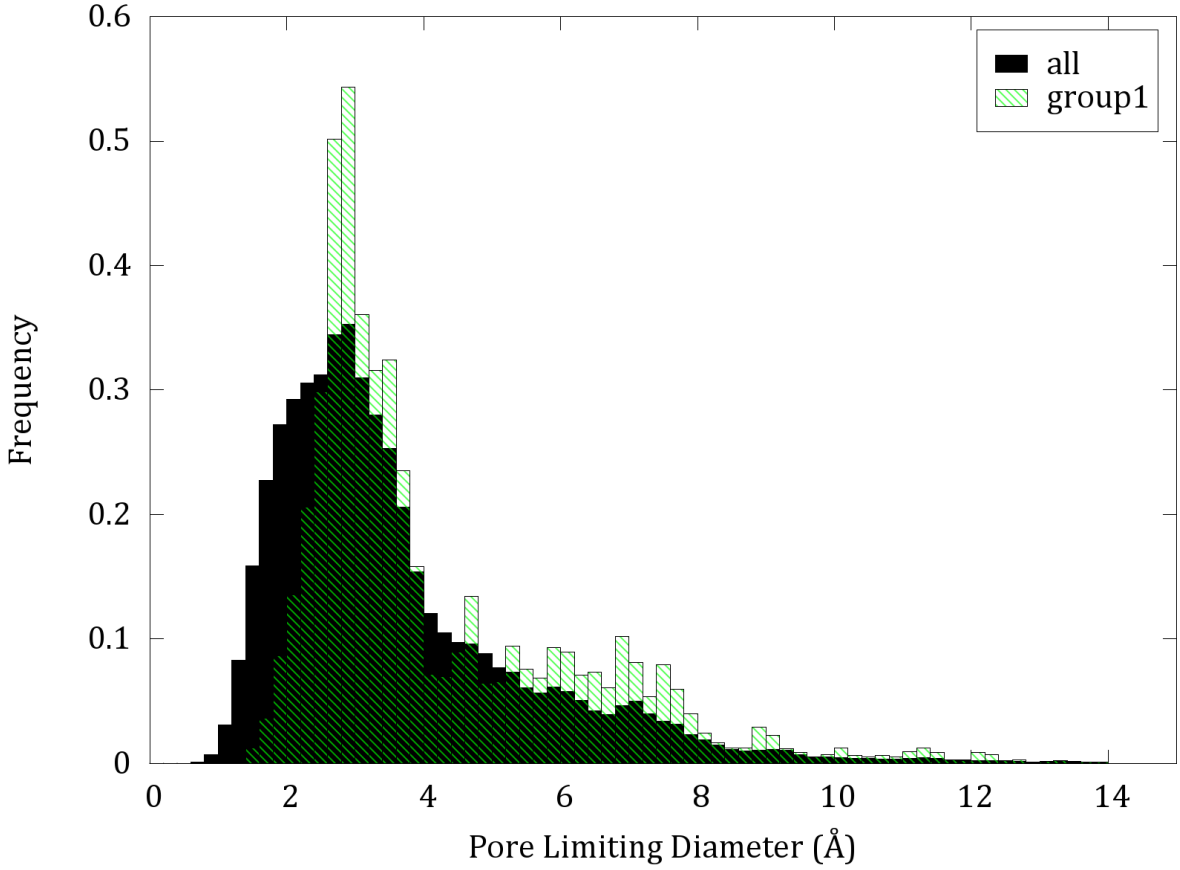

Figure S.3: Histogram showing the frequency of structures for a PLD value for all structures and group 1. The frequency has been normalized so that the histograms give an area of 1.

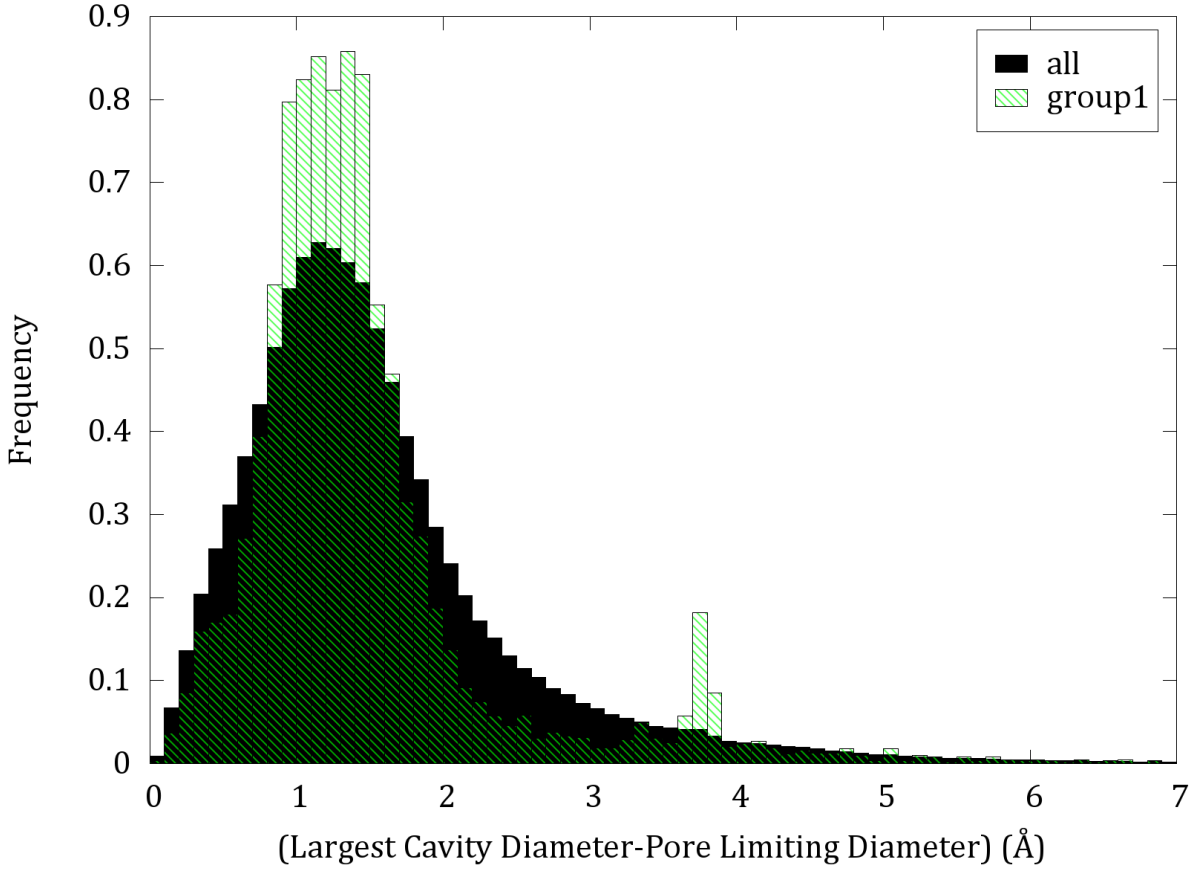

Figure S.4: Histogram showing the frequency of structures with specified values of (LCD-PLD) for all structures and group 1. The frequency has been normalized so that the histograms give an area of 1.

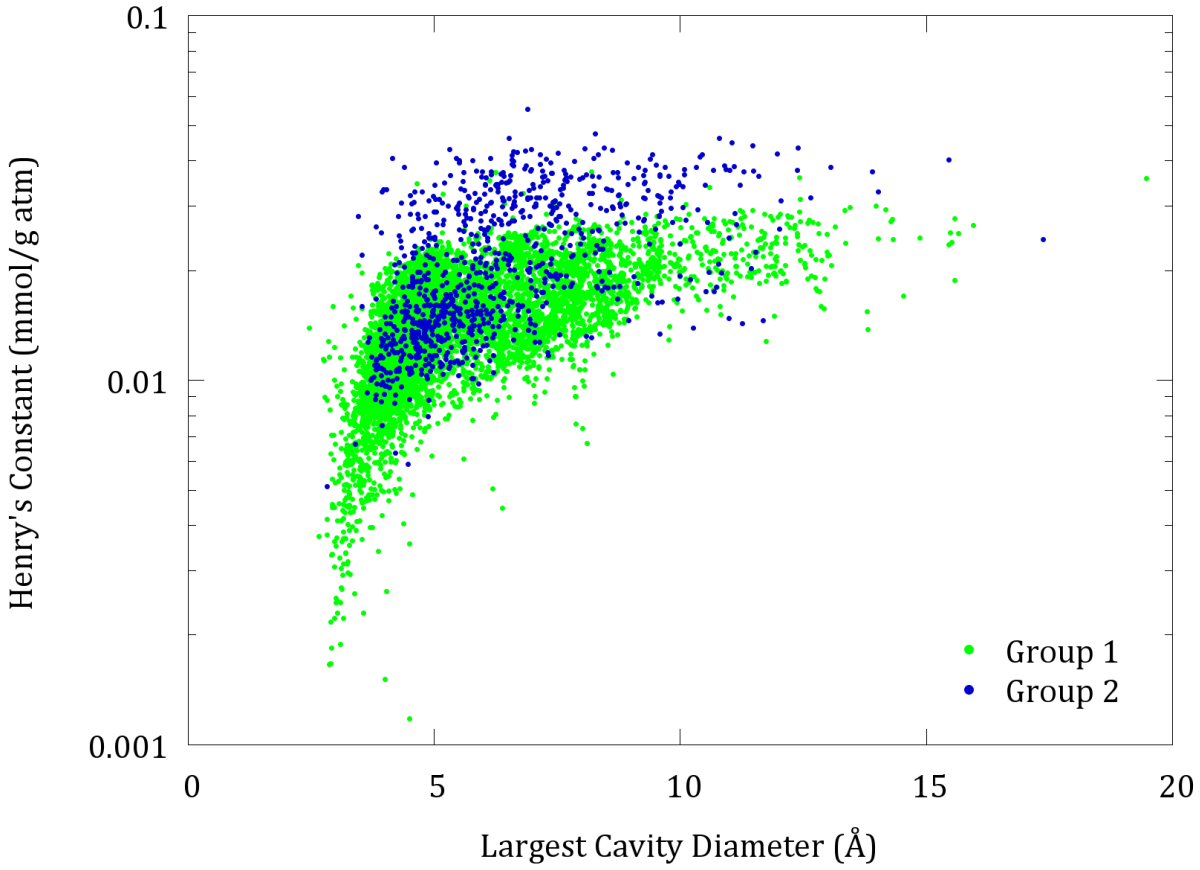

Figure S.5: The Henry's constant for H_2 plotted against the LCD values for the structures in group 1 and group 2.

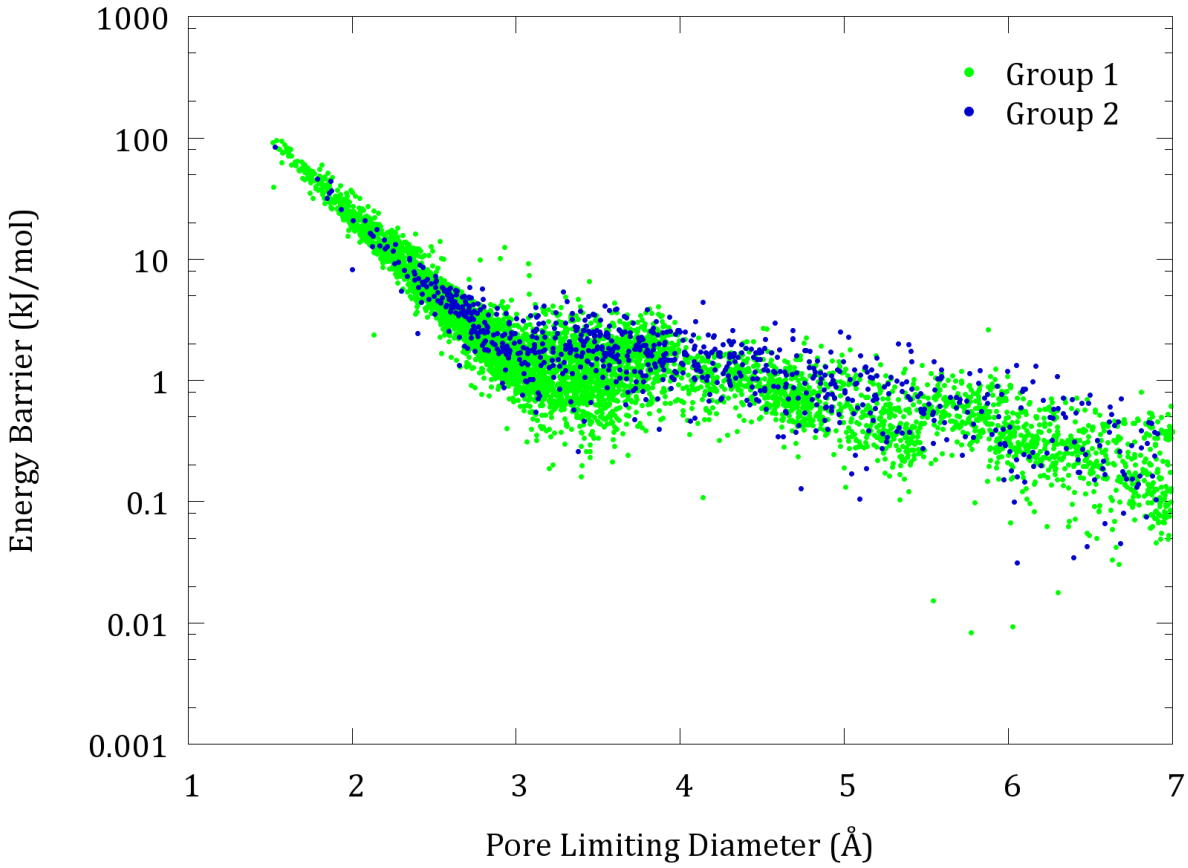

Figure S 6: The energy barrier to diffusion of H_2 plotted against the PLD values for the structures in group 1 and group 2.