

Dynamic Triple-Mode Sorption and Outgassing in Materials

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Table S1: SCE optimized parameters for Sylgard-184 at 30, 40, and 50 °C.

Sn	Parameter	Sylgard-184		
		30 °C	40 °C	50 °C
1	Effective diffusivity (D)	1.202×10^{-3}	1.791×10^{-3}	1.822×10^{-3}
2	Desorption rate (k_s)	1.092×10^{-4}	8.599×10^{-4}	1.001×10^{-5}
3	Langmuir capacity (C'_H)	1.012×10^{-3}	5.539×10^{-2}	1.155×10^{-2}
4	Langmuir affinity (b')	9.502×10^{-1}	1.018×10^{-1}	9.443×10^{-1}
5	Pooling factor (α)	4.831×10^{-1}	4.77×10^{-1}	5.817×10^{-1}
6	Pooling threshold (C_H^0)	4.851×10^{-1}	5.793×10^{-1}	6.228×10^{-1}
7	Pooling power (n)	1.804	2.159	1.839
8	Henry's law constant (k_d)	2.344×10^1	1.484×10^1	1.082×10^1

Table S2: SCE optimized parameters for Zircar RS-1200 at 30, 50, and 70 °C.

Sn	Parameter	Zircar RS-1200		
		30 °C	50 °C	70 °C
1	Effective diffusivity (D)	2.0142×10^{-2}	3.017×10^{-1}	2.08×10^{-2}
2	Desorption rate (k_s)	6.27184×10^{-1}	9.823×10^{-1}	8.655×10^{-1}
3	Langmuir capacity (C'_H)	3.13637	3.075	3.211
4	Langmuir affinity (b')	4.55268	3.739	3.385
5	Pooling factor (α)	5.33525	1.186	1.575
6	Pooling threshold (C_H^0)	4.02646×10^{-1}	6.229×10^{-1}	5.487×10^{-1}
7	Pooling power (n)	3.2268	3.721	4.028
8	Henry's law constant (k_d)	5.5268×10^1	2.914×10^1	1.69×10^1
9	Reduced tortuosity (τ)	1.23×10^{-2}	2.090×10^{-3}	5.627×10^{-2}

Figure S1: probability density plot for error analysis in Sylgard-184. Relative error (computed using $relative\ error = \frac{model\ result - experimental\ data}{experimental\ data}$) is relatively small and centered between $\pm 3\%$ indicative of an excellent match between experiment and simulations as shown in figure below. Analysis corresponds to Fig. 3 in the main text.

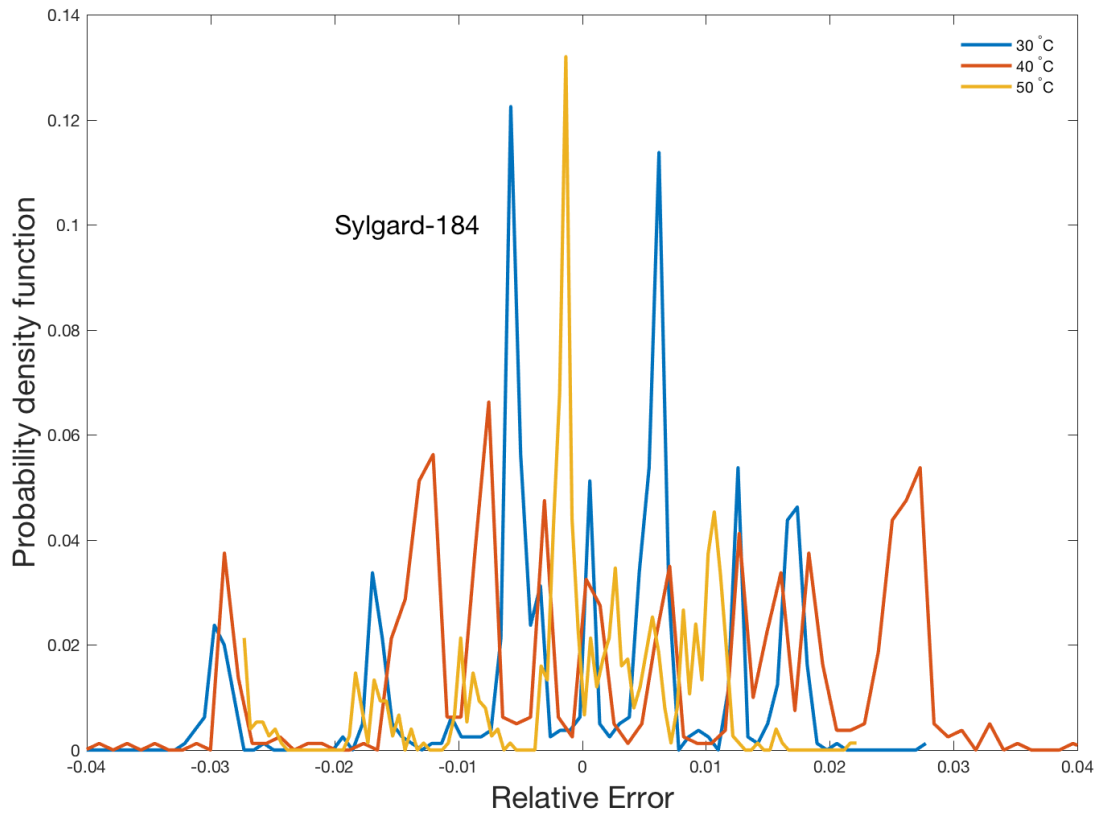
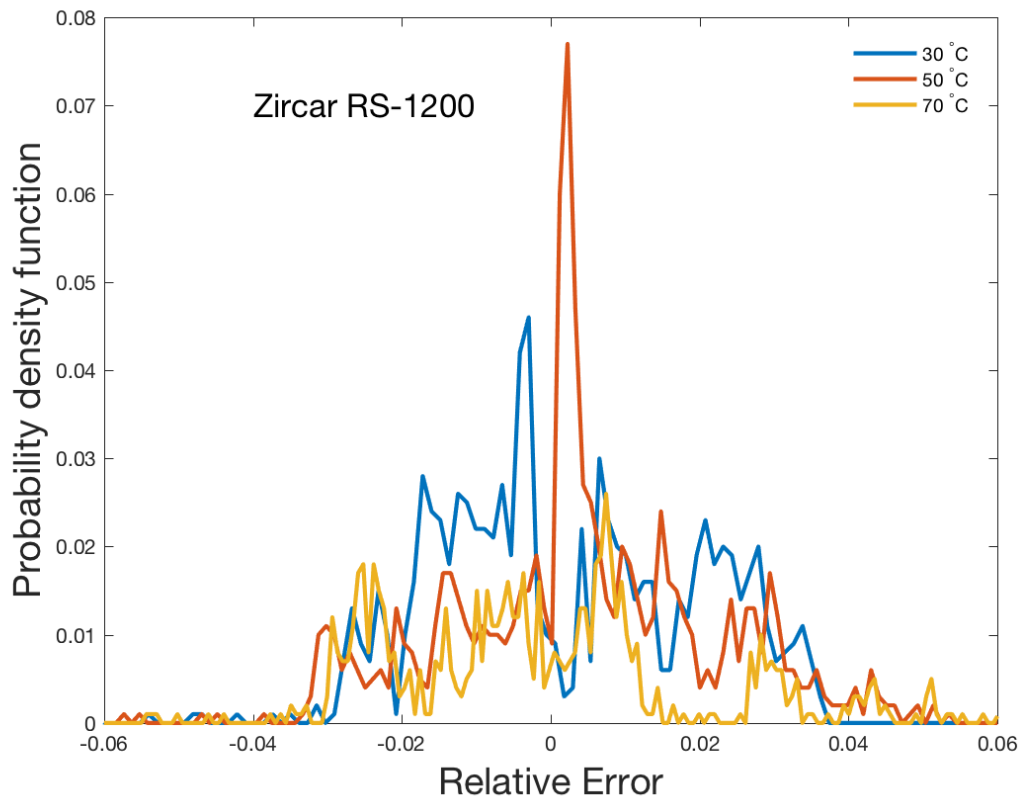
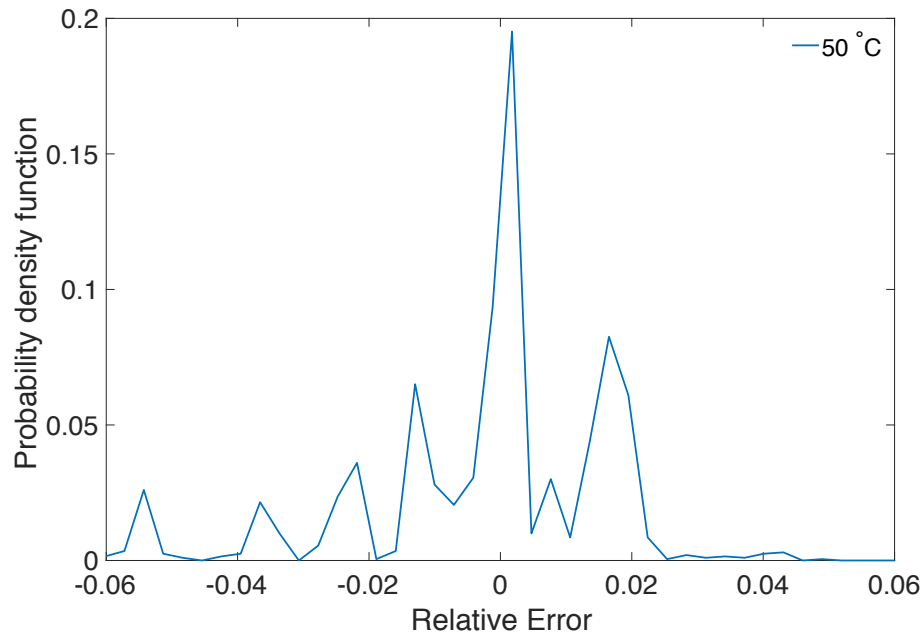


Figure S2: probability density plot for error analysis in Zircar RS-1200 corresponding to Fig. 3 in the main text.



S3: Probability density plot for error analysis in Sylgard-184 at 50 °C corresponding to the experimental data and simulations from Fig 7a in the main text.



S4: Probability density plot for error analysis in Zircar RS-1200 at 50 °C corresponding to the experimental data and simulations from Fig 7b in the main text.

