Supporting Information: An automated multi-scale approach to predict self-diffusion from a potential energy field

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To estimate the statistical error of the computed diffusion coefficients we ran 10 separate simulations with molecular dynamics (MD) and kinetic Monte Carlo (kMC), respectively. Diffusion coefficients were computed for each simulation and the averaged values, $\tilde{D}$, in each direction together with corresponding standard deviations, σD, are presented in table S1. For the IFY structure the diffusive regime is not reached within the time scale of the MD simulation while in the kMC it does where the kMC shows diffusion coefficients at the limit of what can be probed within the MD timescale. Data points of the 4 remaining directional diffusion coefficients (1 from the 1-dimensional diffusion channel PSI structure and 3 from the 3-dimensional AEI) are presented with statistical errors in figure S1. Figures S2–S11 present the mean square displacements (MSD) for all simulations. Figures S2, S3, S6, S8 and S9 present the log-log plots of the MSDs showing that the diffusive regime has been reached when the slope is equal to 1 while

Figures S4, S5, S7, S10 and S11 present the linear plots of the MSDs presented together with the mean square regressed first degree polynomial used to compute the diffusion coefficients presented in table S1 and figure S1. These polynomials are fitted to the data points between the first MSD point passing l^2 and the first point passing $2l^2$ where l is the length of the unit cell in respective direction.

Table S1: Averaged directional diffusion coefficients and standard deviations for structures PSI, IFY and AEI. Data is presented in cm^2/s.

	$\tilde{D}_x$	σD_x	$\tilde{D}_y$	σD_y	$\tilde{D}_z$	σD_z
AEI kMC	2.8e-6	0.7e-6	5.0e-7	2.6e-7	7.9e-7	3.9e-7
AEI MD	3.5e-6	0.8e-6	3.0e-6	0.6e-6	2.7e-6	1.4e-6
IFY kMC	7.5e-7	1.9e-7	7.2e-7	1.3e-7	0	0
IFY MD	0	0	0	0	0	0
PSI kMC	1.85e-4	0.01e-4	0	0	0	0
PSI MD	2.4e-5	0.3e-5	0	0	0	0

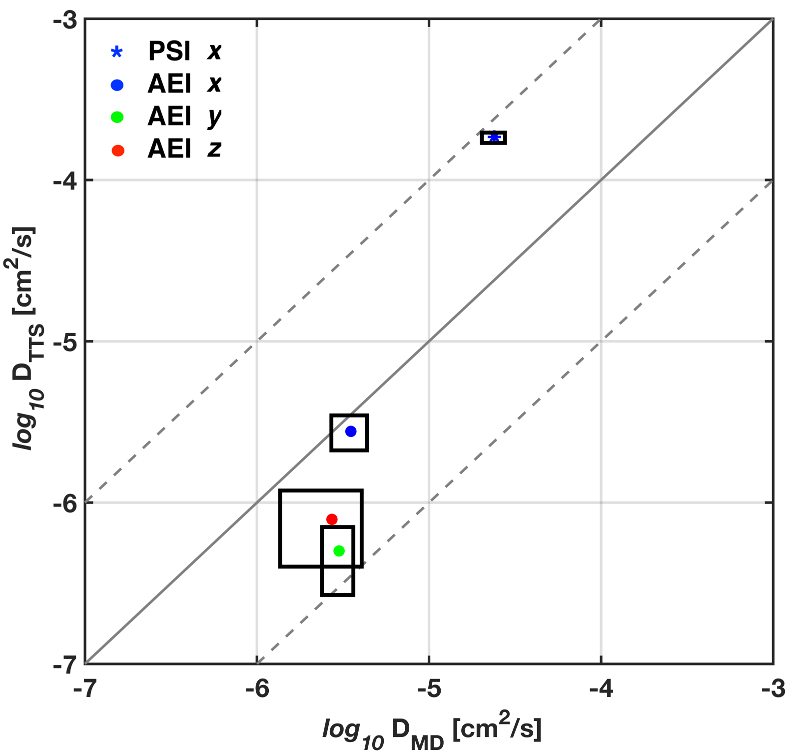

Figure S1: Markers present averaged directional diffusion coefficients computed from MD as compared to those computed with kMC. The standard deviations are represented by black boxes surrounding the respective markers. The solid grey line represents a perfect correspondence between the MD and kMC data while the grey dashed lines guide the limits for the deviation of 1 order of magnitude.

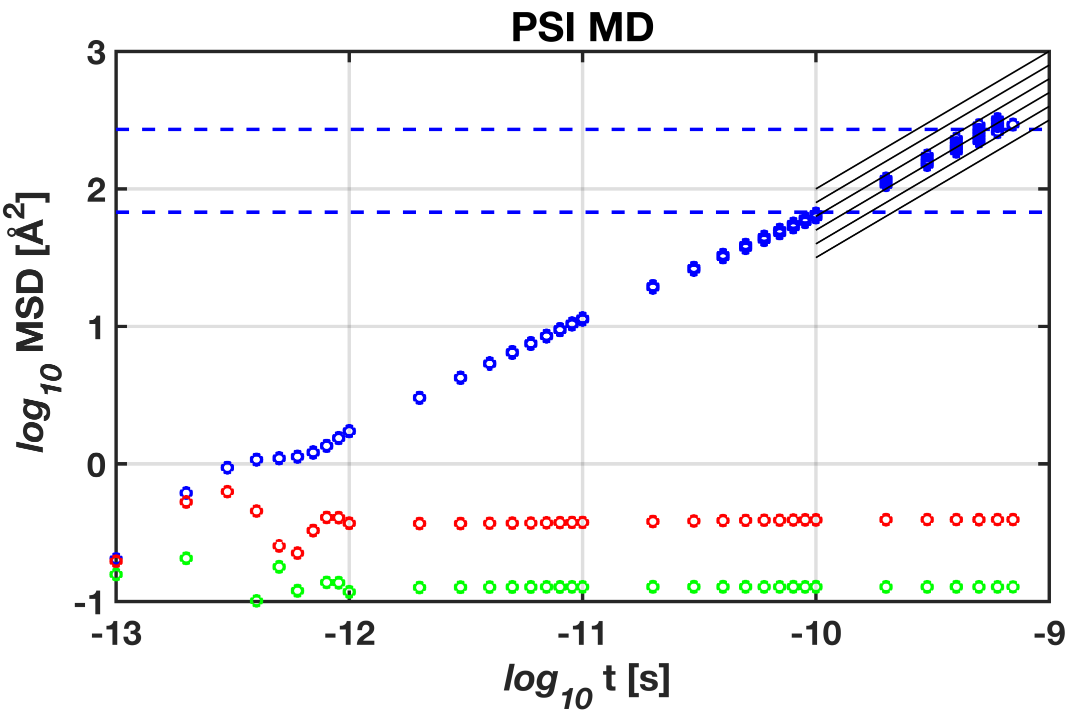

Figure S2: Log-log plots of the MD MSD (is x=blue, y=green, x=red) as a function of time. The black solid lines represent slopes equaling 1 confirming the diffusive regime of the MSD. The horizontal dashed lines represent l^2 and $2l^2$ for diffusive directions in respective color.

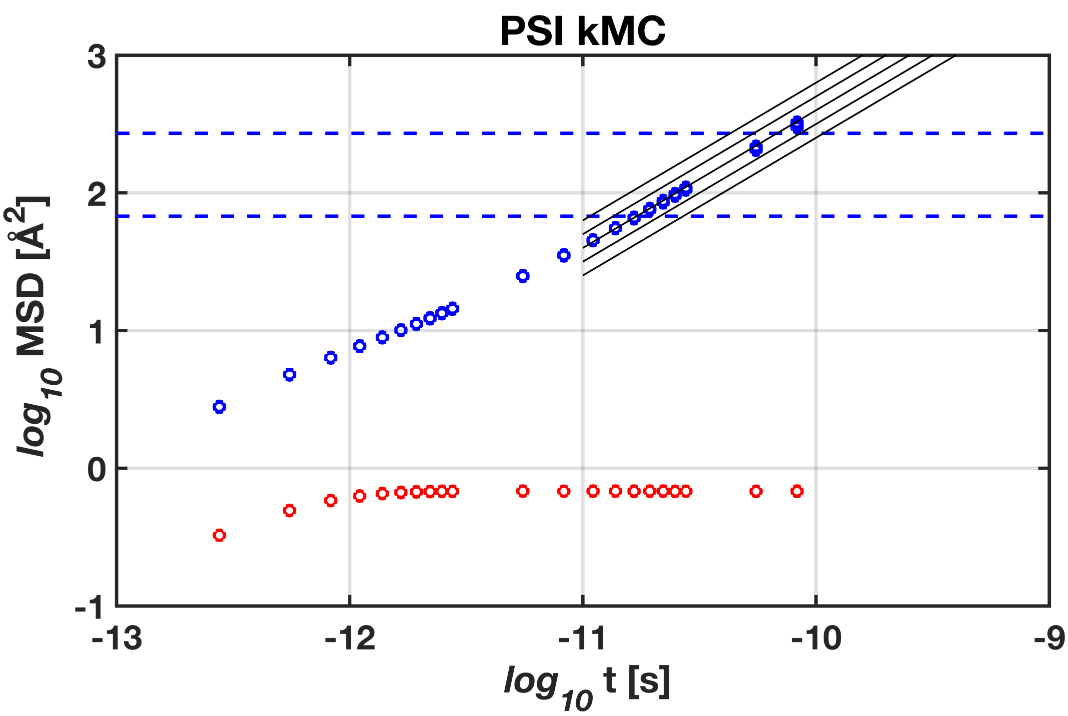

Figure S3: Log-log plots of the kMC MSD (is x = blue, z = red) as a function of time. The black solid lines represent slopes equaling 1 confirming the diffusive regime of the MSD. The horizontal dashed lines represent l^2 and $2l^2$ for diffusive directions in respective color. The MSD curve for the y-direction is in the range of 10^{-3} and outside the plotted region.

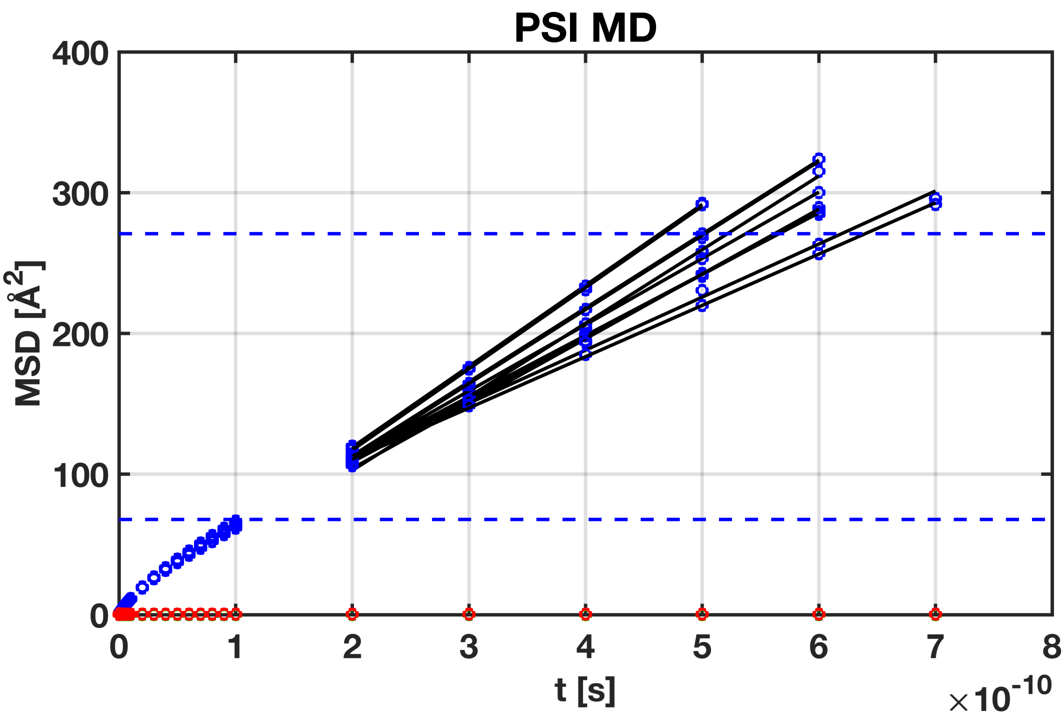

Figure S4: Linear plots of the MD MSD (is x = blue, y, z = red) as a function of time. The black lines represent the 1st degree polynomials fitted to each MSD curve. The horizontal dashed lines represent l^2 and $2l^2$ for diffusive directions in respective color.

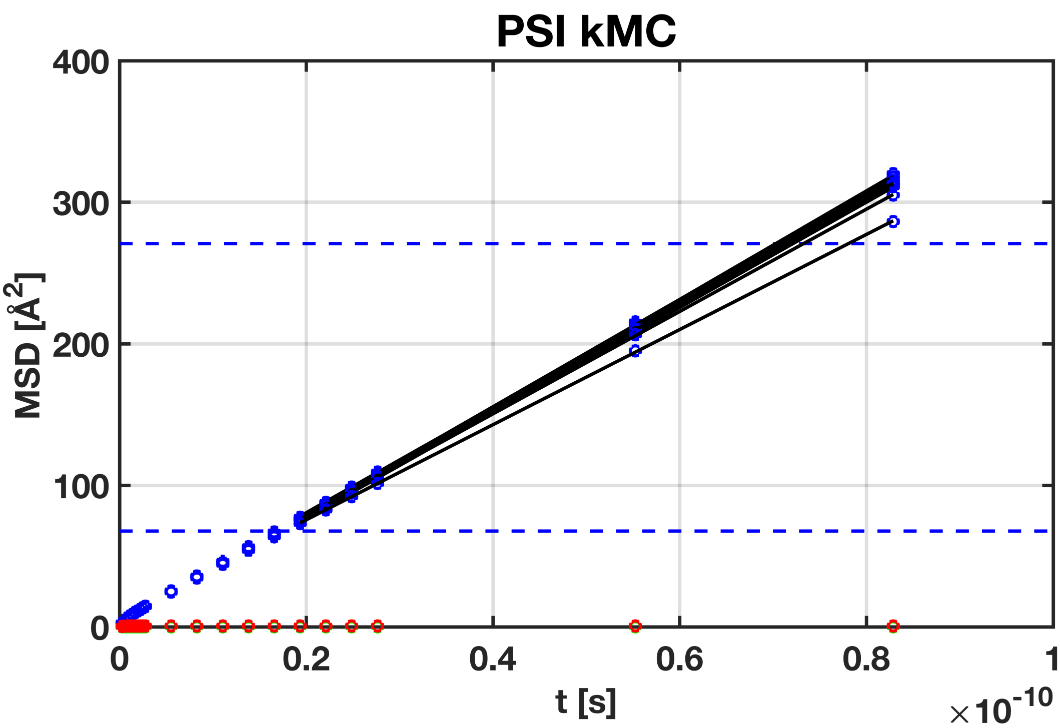

Figure S5: Linear plots of the kMC MSD (is x =blue, y, z = red) as a function of time. The black lines represent the 1st degree polynomials fitted to each MSD curve. The horizontal dashed lines represent l^2 and $2l^2$ for diffusive directions in respective color.

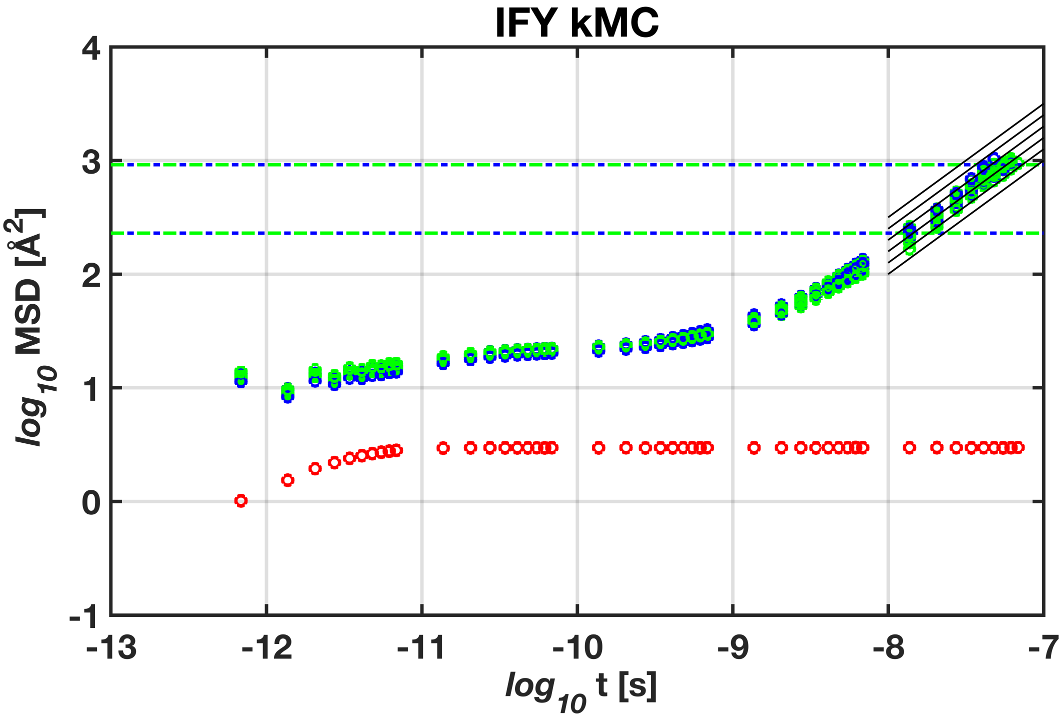

Figure S6: Log-log plots of the kMC MSD (is x = blue, y = green, z = red) as a function of time. The black solid lines represent slopes equaling 1 confirming the diffusive regime of the MSD. The horizontal dashed lines represent l^2 and $2l^2$ for diffusive directions in respective color.

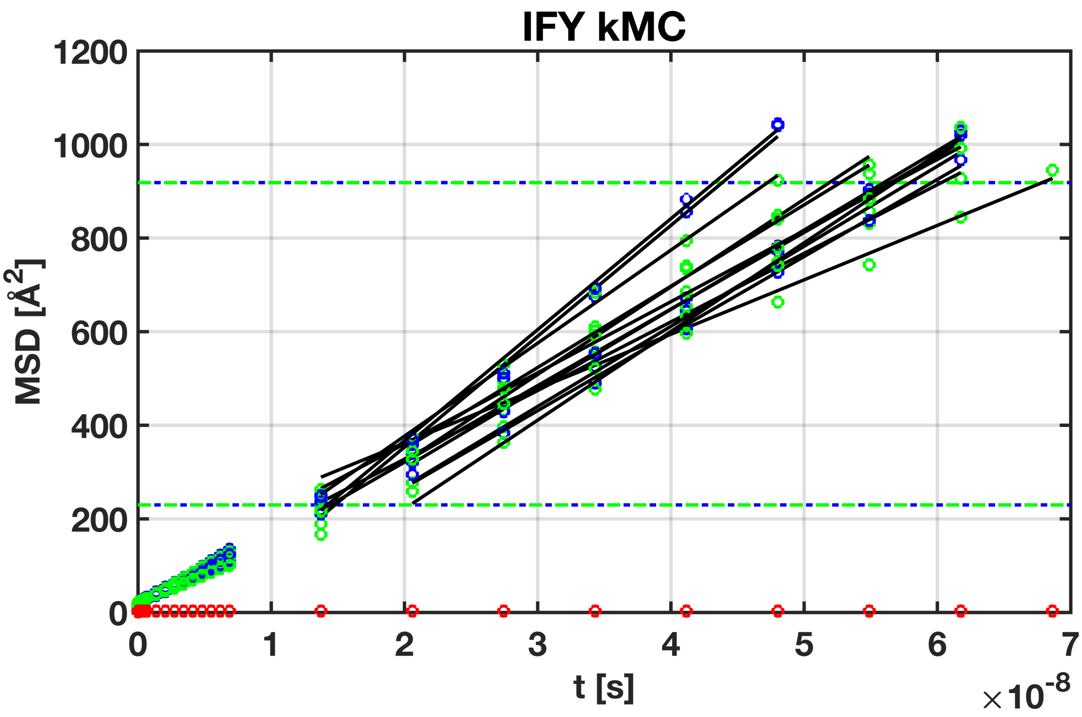

Figure S7: Linear plots of the kMC MSD (is x = blue, y = green, z = red) as a function of time. The black lines represent the 1st degree polynomials fitted to each MSD curve. The horizontal dashed lines represent l^2 and $2l^2$ for diffusive directions in respective color.

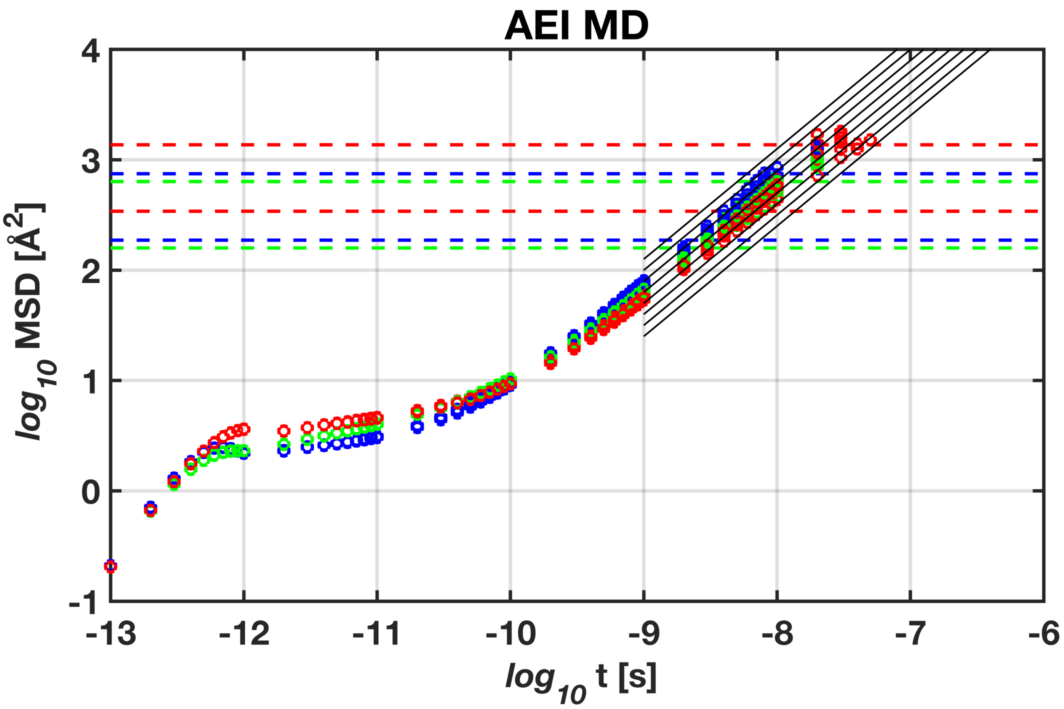

Figure S8: Log-log plots of the MD MSD (is x = blue, y = green, z = red) as a function of time. The black solid lines represent slopes equaling 1 confirming the diffusive regime of the MSD. The horizontal dashed lines represent l^2 and $2l^2$ for diffusive directions in respective color.

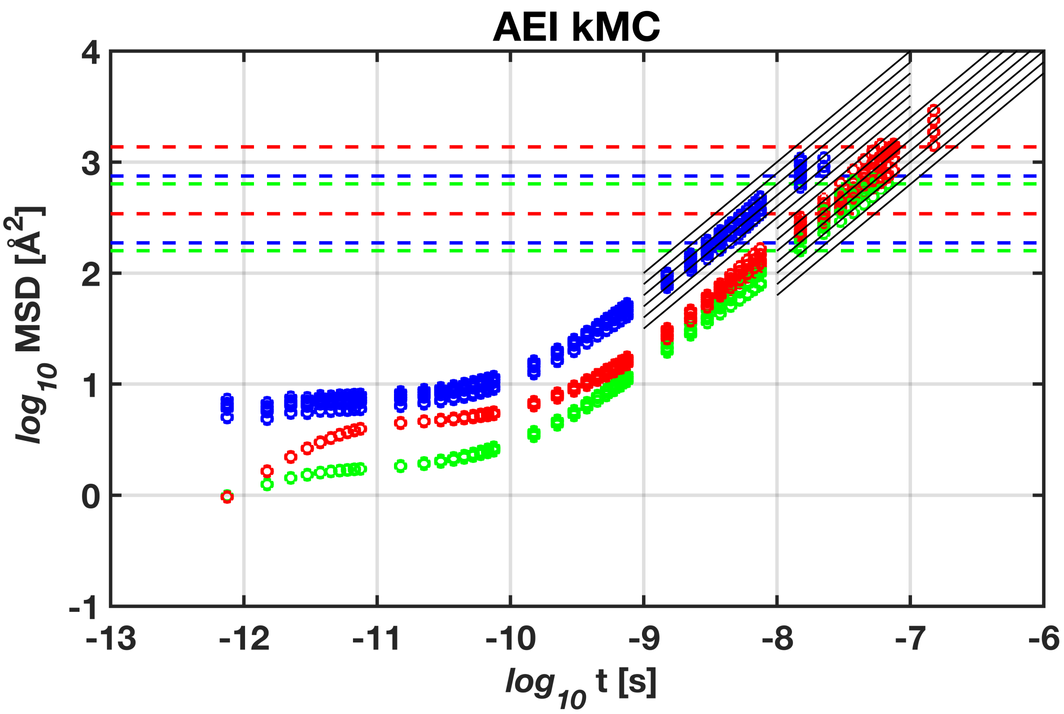

Figure S9: Log-log plots of the kMC MSD (is x = blue, y = green, z = red) as a function of time. The black solid lines represent slopes equaling 1 confirming the diffusive regime of the MSD. The horizontal dashed lines represent l^2 and $2l^2$ for diffusive directions in respective color.

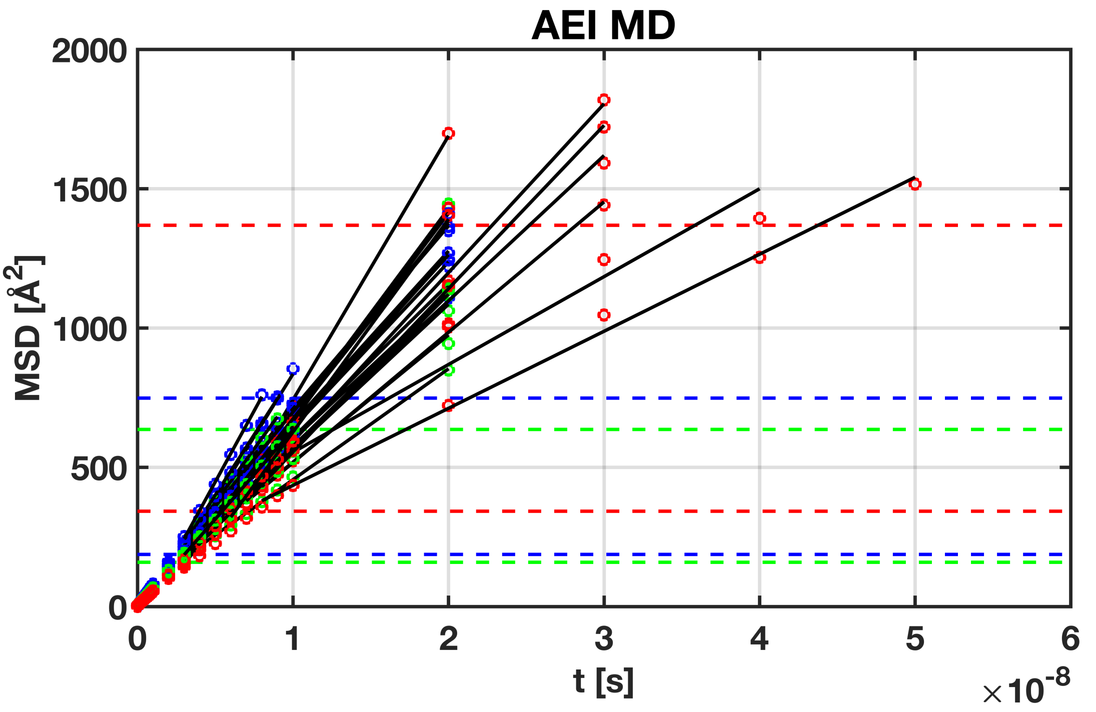

Figure S10: Linear plots of the MD MSD (is x = blue, y = green, z = red) as a function of time. The black lines represent the 1st degree polynomials fitted to each MSD curve. The horizontal dashed lines represent l^2 and $2l^2$ for diffusive directions in respective color.

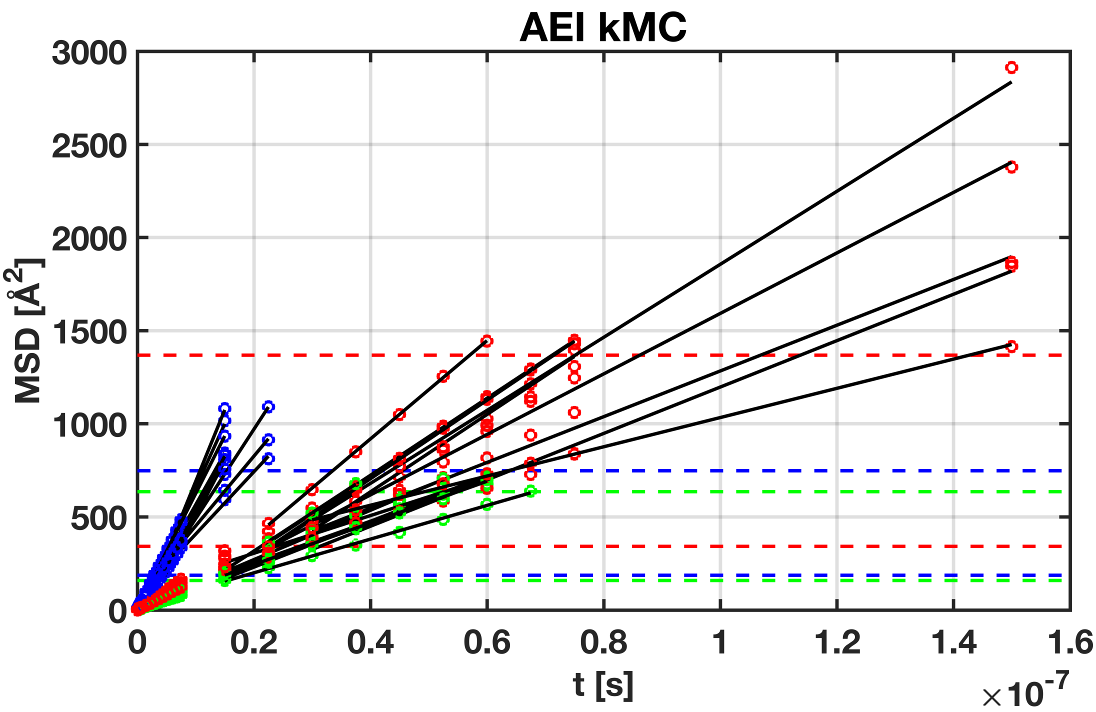

Figure S11: Linear plots of the kMC MSD (is x = blue, y = green, z = red) as a function of time. The black lines represent the 1st degree polynomials fitted to each MSD curve. The horizontal dashed lines represent l^2 and $2l^2$ for diffusive directions in respective color.