

Supplementary Information for Machine Learning-Driven Investigation of the Structure and Dynamics of the BMIM-BF₄ Room Temperature Ionic Liquid

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Radial distribution functions

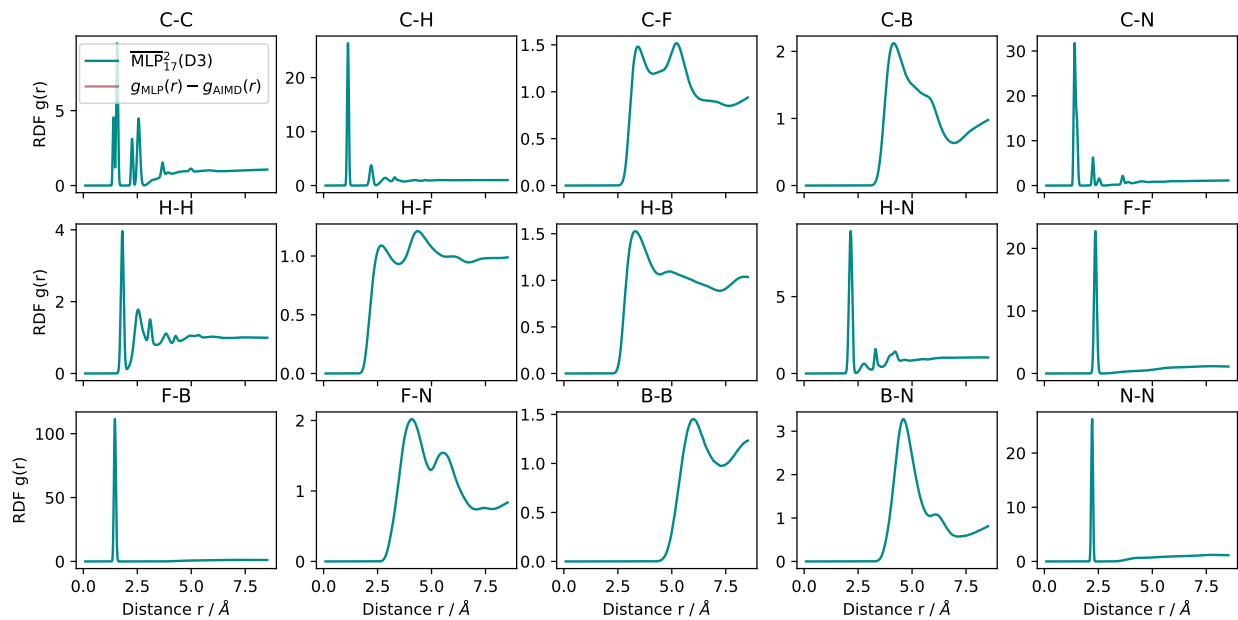


Figure S1: radial distribution function (RDF) for 16 ion pairs at 283 K.

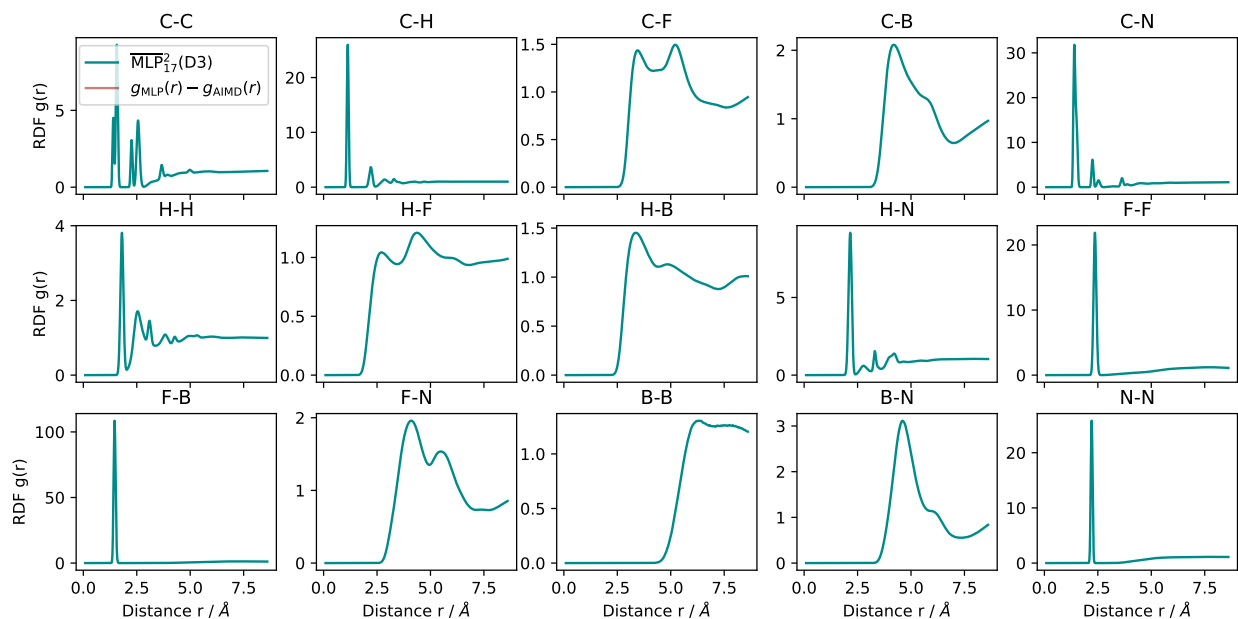


Figure S2: RDF for 16 ion pairs at 293 K.

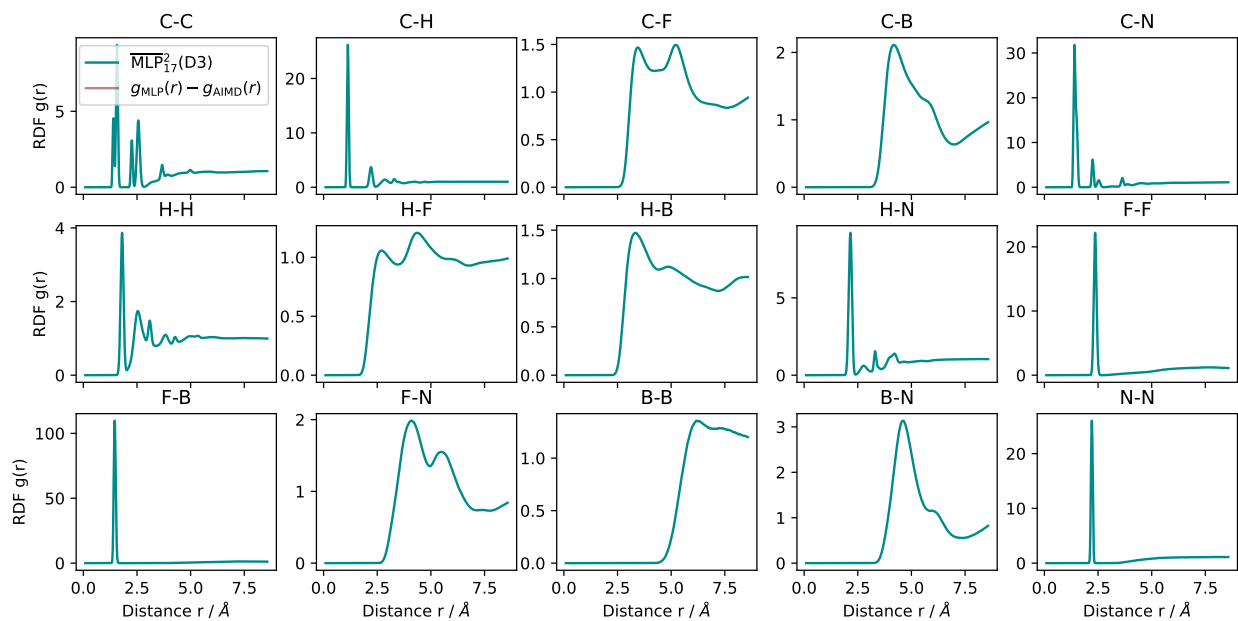


Figure S3: RDF for 16 ion pairs at 313 K.

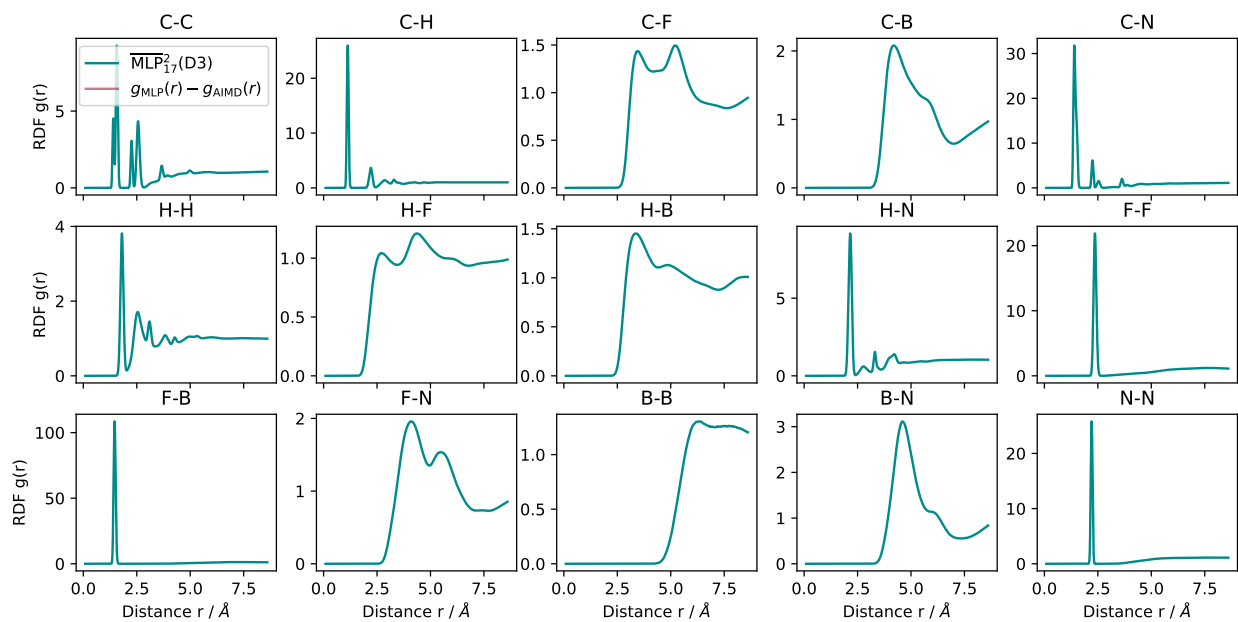


Figure S4: RDF for 16 ion pairs at 333 K.

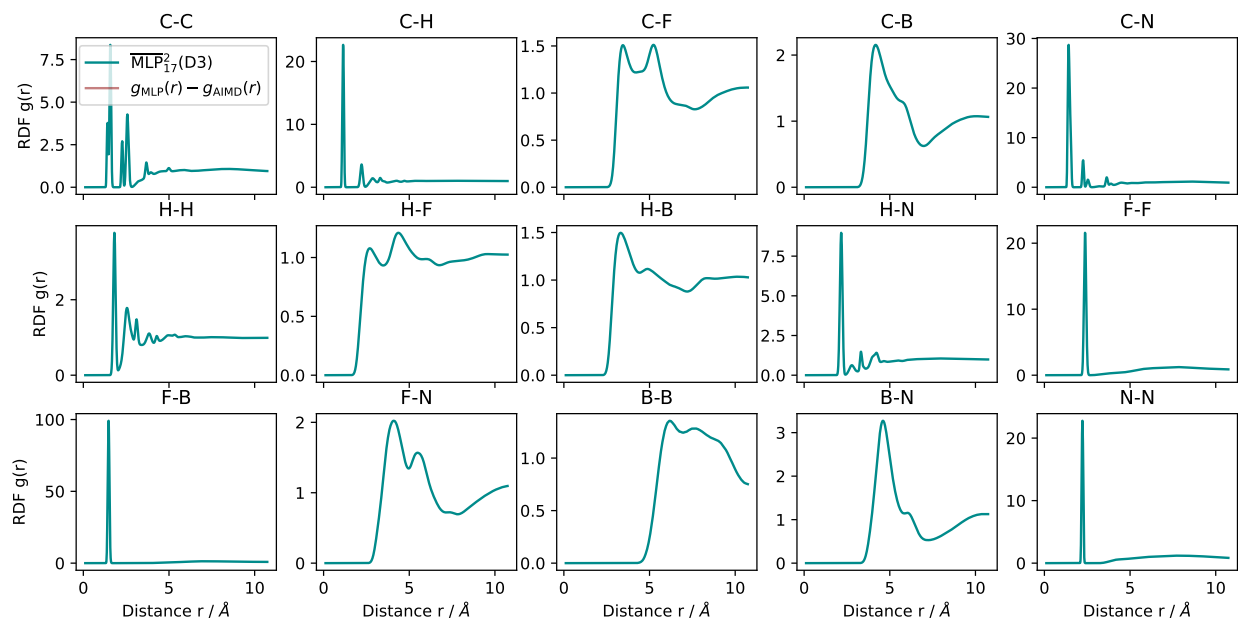


Figure S5: RDF for 32 ion pairs at 283 K.

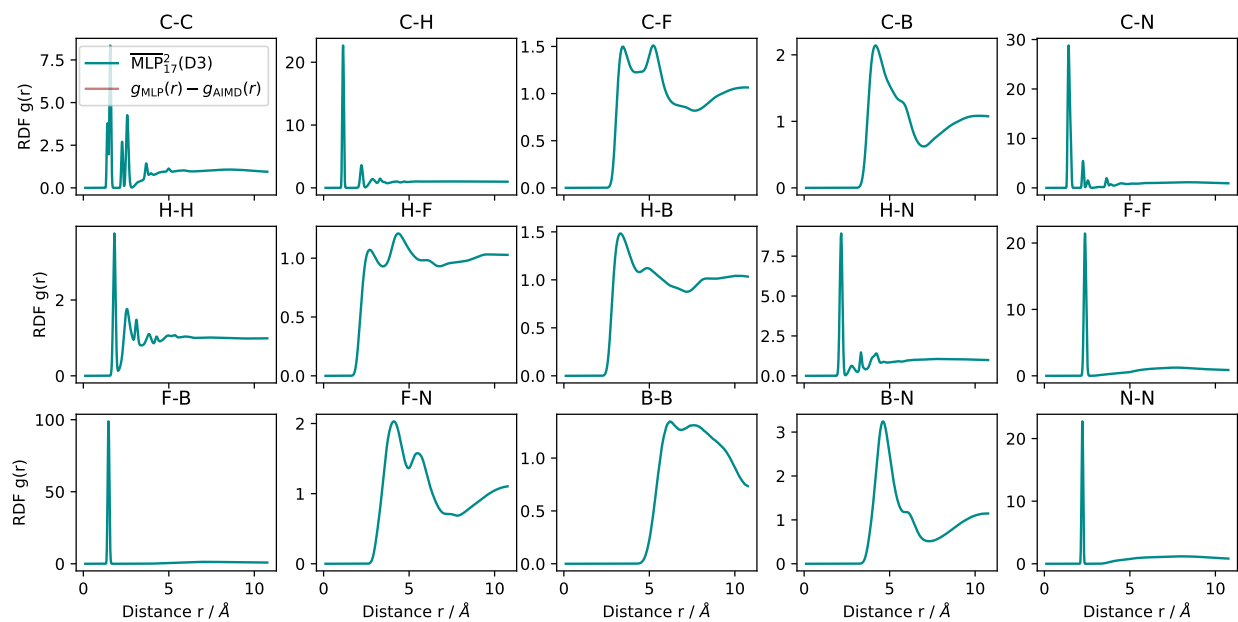


Figure S6: RDF for 32 ion pairs at 293 K.

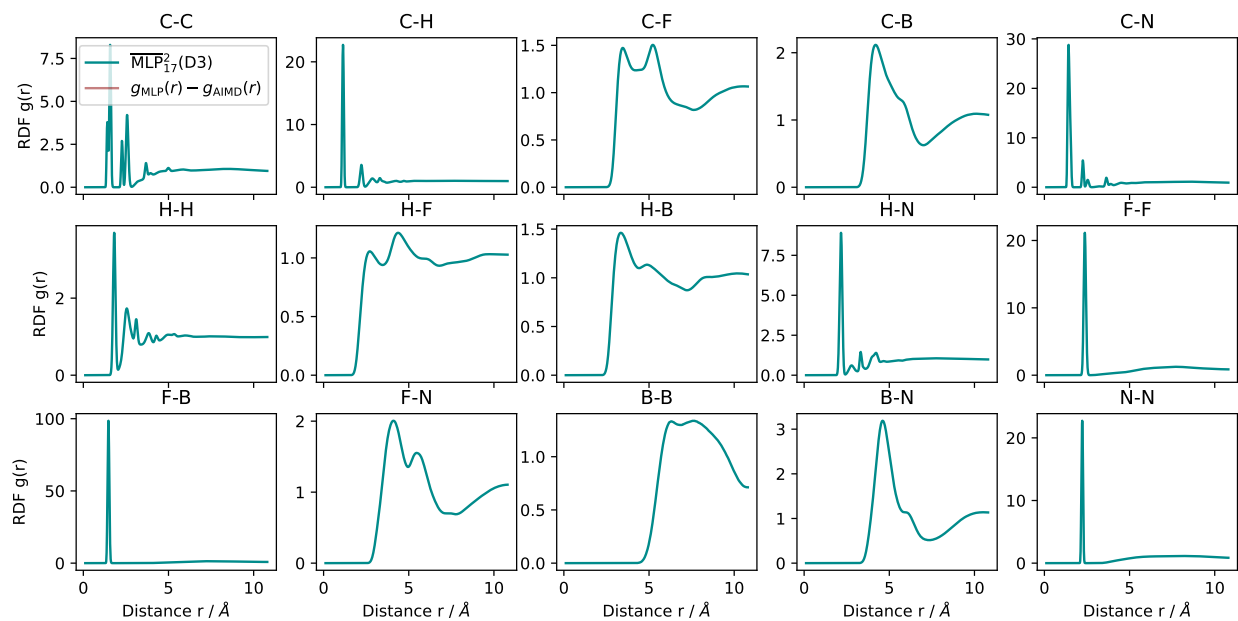


Figure S7: RDF for 32 ion pairs at 313 K.

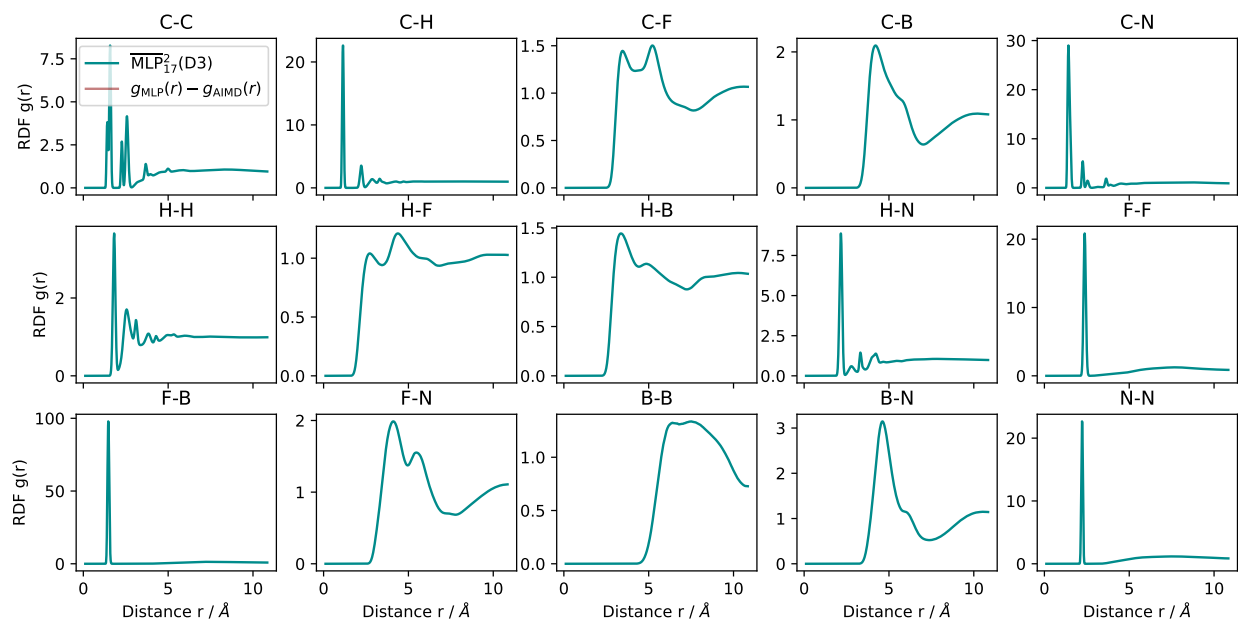


Figure S8: RDF for 32 ion pairs at 333 K.

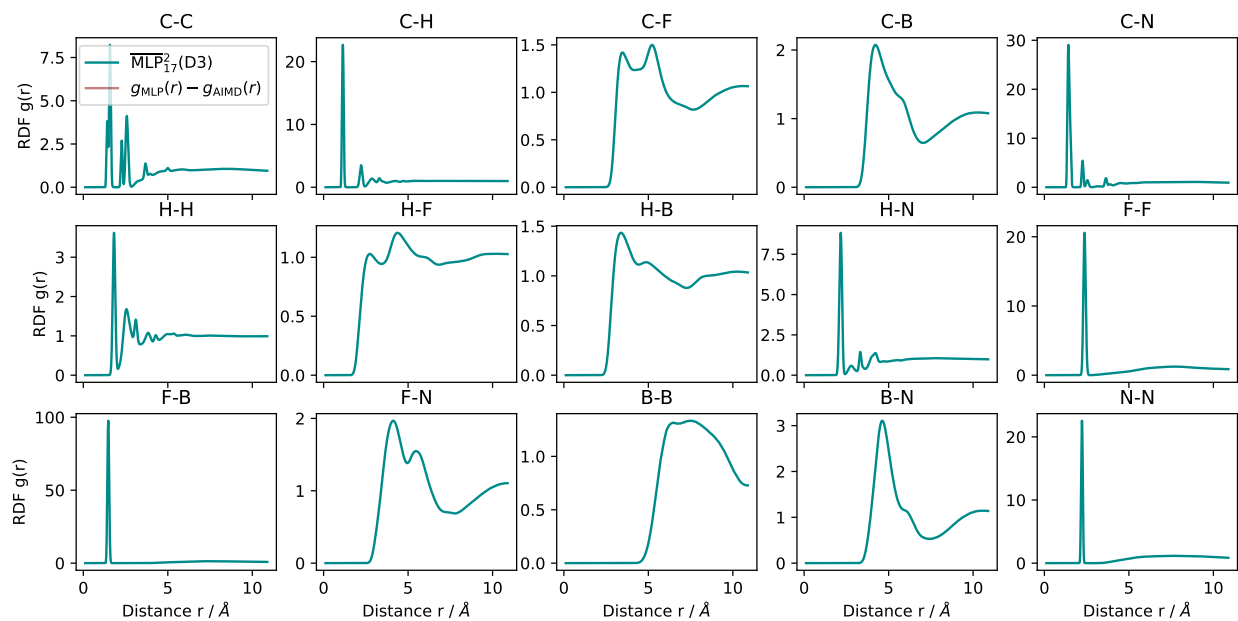


Figure S9: RDF for 32 ion pairs at 353 K.

Diffusion coefficients

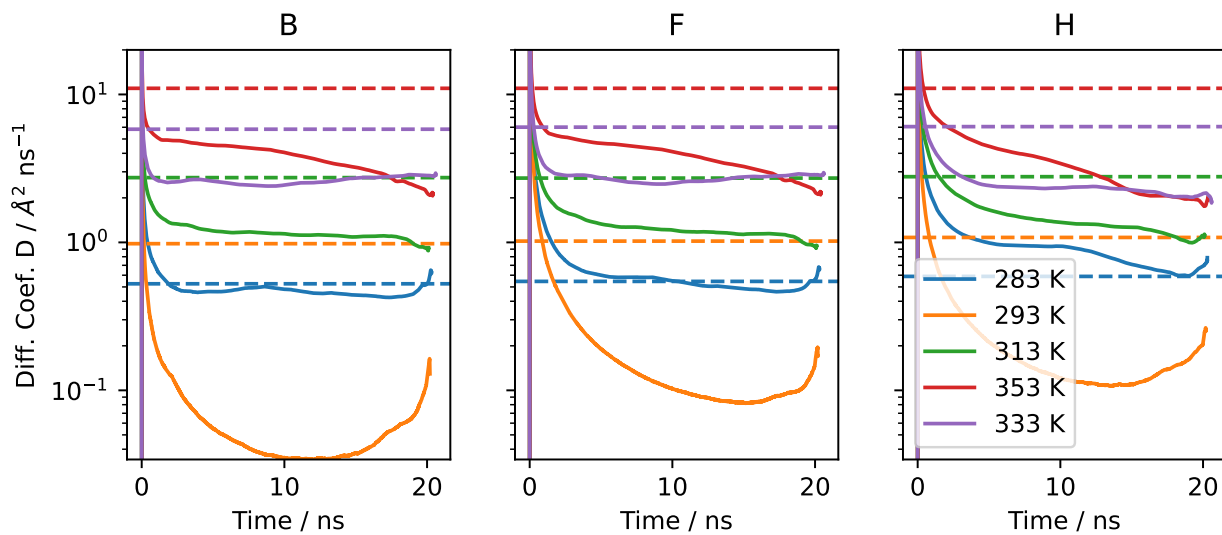


Figure S10: Diffusion coefficients for 8 ion pairs at different temperatures compared to literature.

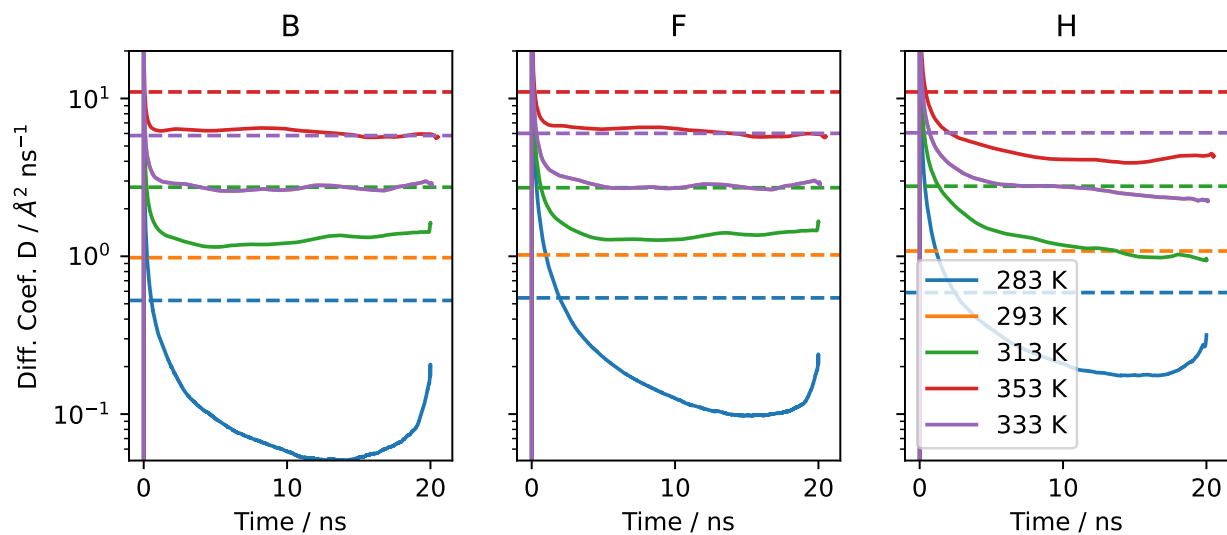


Figure S11: Diffusion coefficients for 16 ion pairs at different temperatures compared to literature.

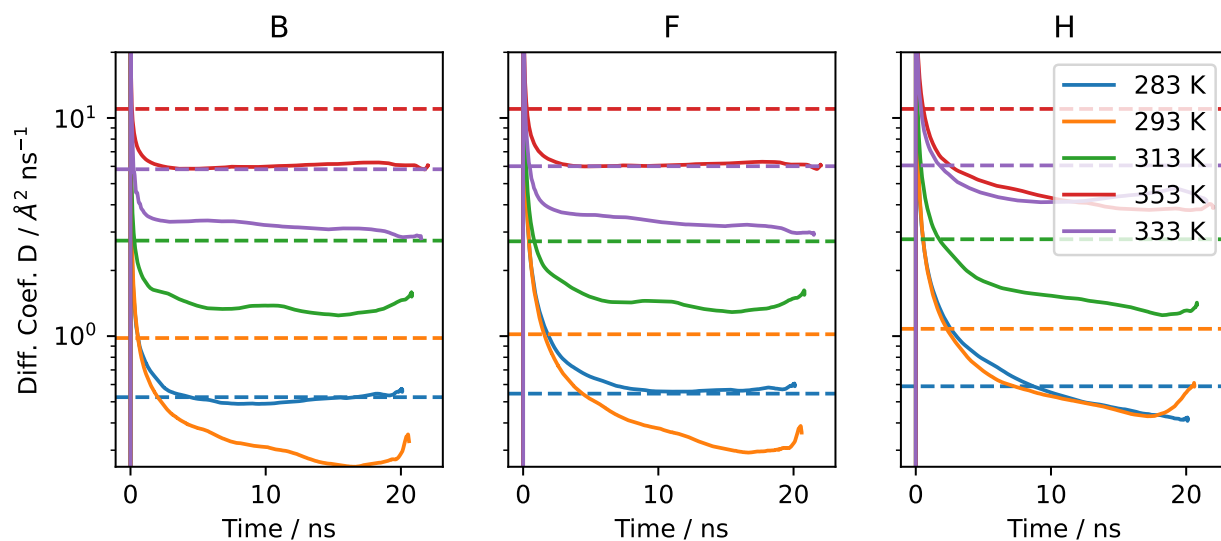


Figure S12: Diffusion coefficients for 32 ion pairs at different temperatures compared to literature.

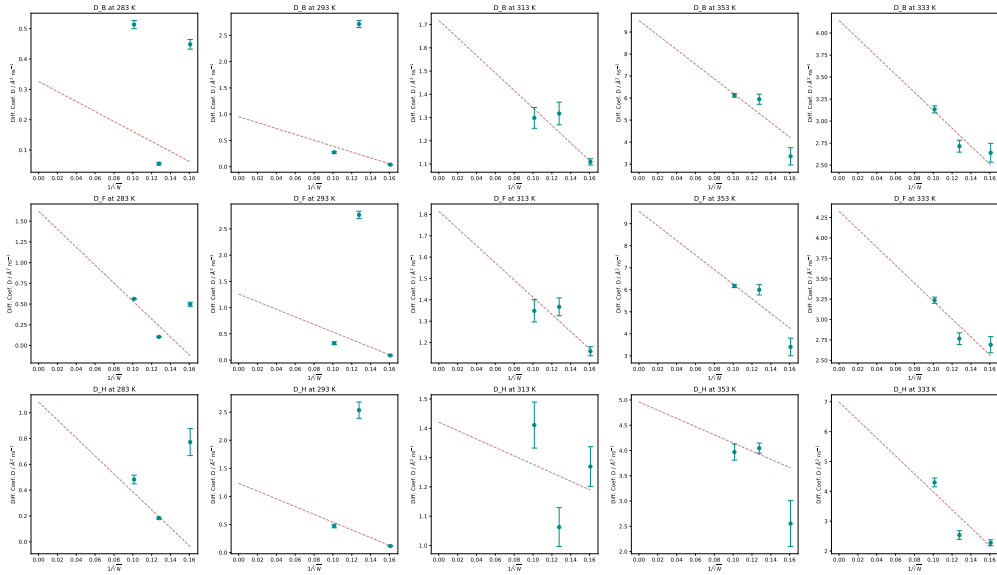


Figure S13: Finite size scaling of the diffusion coefficients.

Density

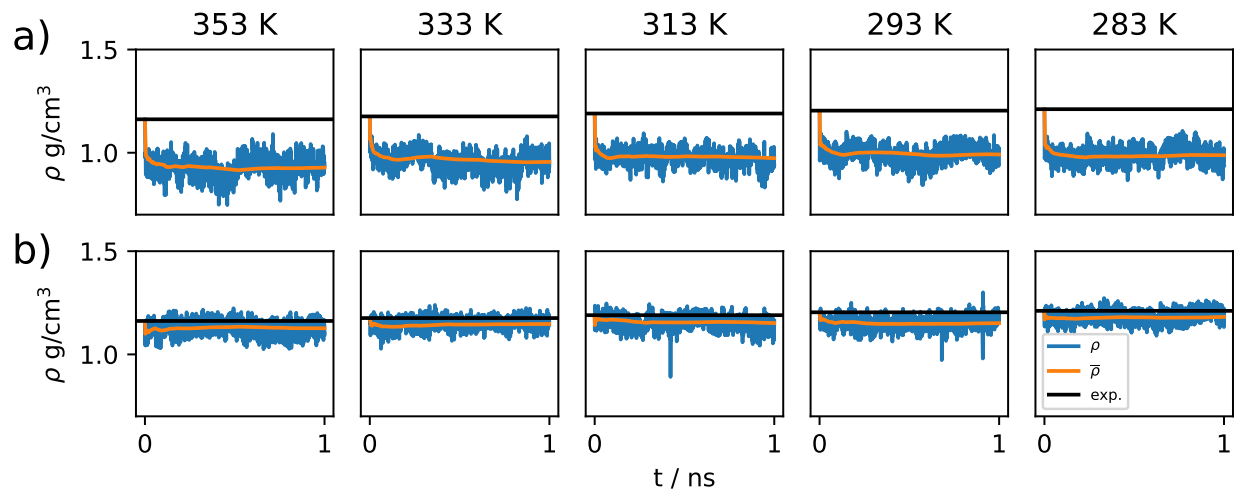


Figure S14: Density over time for a) $\overline{\text{MLP}}_{17}^2(\text{D3}(8 \text{ \AA}))$ and b) $\overline{\text{MLP}}_{17}^2+\text{D3}(20 \text{ \AA})$

AIMD

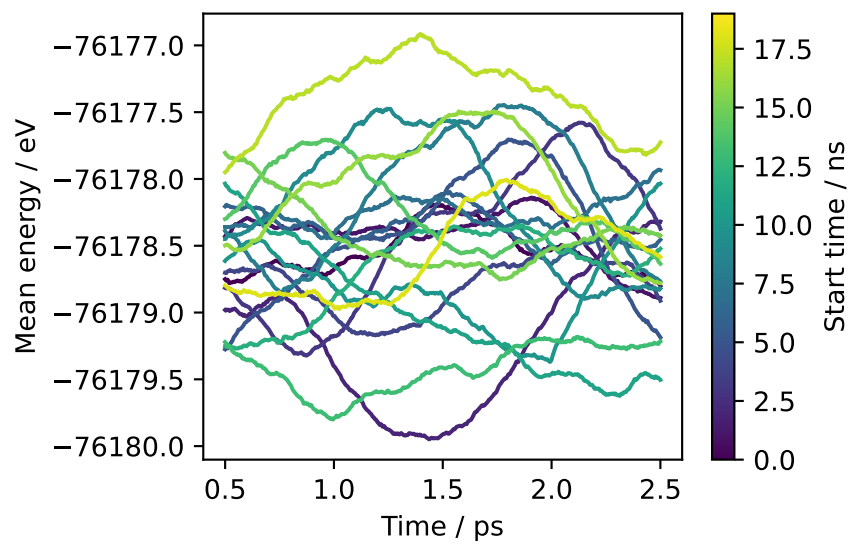


Figure S15: Energies of the 20×2.5 ps *ab initio* molecular dynamics (AIMD) simulation at 353 K for 16 ion pairs. A running average over 0.5 ps is applied.