DETERMINING THE MELTING POINT OF BIOCOMPATIBLE IONIC LIQUIDS WITH MOLECULAR DYNAMICS SIMULATIONS

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Ionic liquids (ILs) are often promoted as green solvents, while most common ionic liquids were found to be toxic and harmful to the environment [1]. ILs containing choline cation have exhibited remarkably low toxicity, especially in combination with biocompatible anions derived from e.g. carboxylic acids or benzoic acids [2].

However, the primary drawback of such, more biocompatible, ILs is high melting point and poor charge transport properties [2]. Computational chemistry is a useful tool for identifying the ILs with relatively lower melting points as there are many possible cation-anion combinations of biocompatible ILs. The best performing IL melting point prediction methods require experimental crystal structure data, which is scarce for ILs [3].

The current work introduces a computational method to predict the melting points of biocompatible ILs without the prior knowledge of their crystal structure. Solid phases for each IL were constructed in molecular dynamics simulations by using differently packed Coulombic potential wells. Melting point was then determined by irregular change in diffusion coefficient during simulated annealing (Fig. 1). This method was used to predict the melting points of 15 biocompatible ILs.

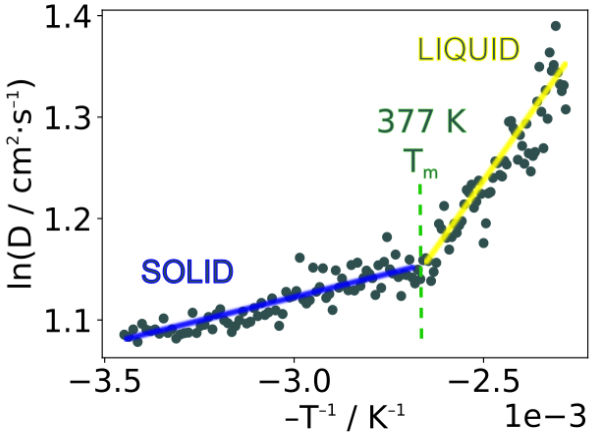

Fig.1 Diffusion coefficient – inverse temperature dependence during simulated annealing.

References

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