Ionic liquid conductivity modelled by machine learning and symbolic regression

Isak Bengtsson[a] and Patrik Johansson[a,b,c,*]

[a]*Department of Physics, Chalmers University of Technology, 412 96 Gothenburg, Sweden*
[b]*Department of Chemistry – Ångström, Uppsala University, 751 21 Uppsala, Sweden*
[c]*Alistore-ERI CNRS FR 3104, 15 Rue Baudelocque, 80039 Amiens, France*
*patrik.johansson@chalmers.se

High thermal stabilities, wide electrochemical stability windows, and especially their inherent ionicities and conductivities make ionic liquids (ILs) promising as components in modern battery electrolytes beyond today's state-of-the-art. They could resolve issues of flammability, unwanted side reactions, and even dissolution of electroactive material[1]. But how to know what IL to choose?

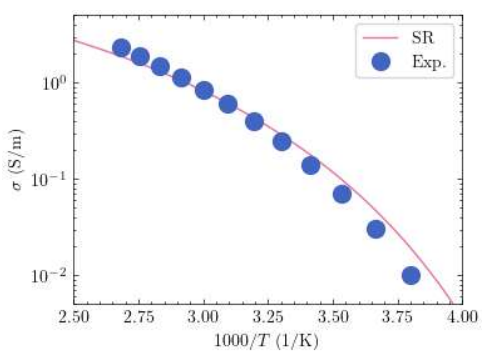

Figure 1: The SR prediction and experimental ionic conductivity data for [C4py][BF4].

Given the vast chemical space of ILs, quoted as >10^{18} unique compositions[2], machine learning (ML) methods offer an efficient and scalable approach[3]. Here we use the ML method symbolic regression (SR) to derive analytical models that describe the ionic conductivity (σ) of >450 aprotic ILs, using molecular descriptors as variables. On the assumption that ion diffusion is related to the amount of free space between species, the model search has been guided towards equations reminiscent of those of free volume theory[4]. One example is:

$$\sigma = \frac{p_0 e^{\frac{I_a \gamma_a - \beta_a(\mu_a + \gamma_c(G_a + p_1) + p_2)}{\beta_a\left(T\,\epsilon_c^{p_3 - \epsilon_a} + p_4\right)}}}{\sqrt{T}},$$

with a function based on the inertial shape factor I, radius of gyration γ, Gini coefficient G, charge variance β, dipole moment μ and the temperature T, showcased for the IL [C4py][BF_4] (Fig. 1). While the temperature trend is captured well for most ILs, the predictions are sometimes shifted by a constant, which could be a consequence of data uncertainties, inconsistencies in the measurement setups, or water contamination. Therefore, in the future, we will use data sourced from a single lab.

References

1. Watanabe, M.; Thomas, M.L.* *Chem. Rev*. **2017**, *117*, 7190–7239.
2. Plechkova, N.; Seddon, K. *Chem. Soc. Rev.* **2008**, *37*, 123-150.
3. Baskin, I.; Epshtein, A.* *J. Mol. Liq.* **2022**, *351*, 118616.
4. Beichel, W.; Yang, Y.* *Phys. Chem. Chem. Phys.* **2013**, *15,* 8821.

I, Isak Bengtsson, received my M.Sc. in Physics from Chalmers University of Technology and started my PhD in the division of Materials Physics in July 2024. My focus is computational physics, especially data-driven methods applied to modelling of ionic liquids and electrolytes to nurture fundamental understanding of properties of these materials.