Quantitative Structure–Property Relationship approach to estimate the α-relaxation dynamics of molecular glass-formers

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The Glass Transition Temperature (T_g) is one of the key properties of interest when developing brand-new materials. It is associated with a sudden change of the dynamic properties of a compound, concerning in particular its relaxation time. Broadband Dielectric Spectroscopy (BDS) is the most extended technique to measure the relaxation time of a compound, by perturbating the system on a wide range of frequencies. Although this characterization is only possible after synthesizing the new materials, recent advances in the computational calculus, in particular Quantitative Structure–Property Relationship models (QSPRs), are becoming valid tools in the estimation of the physical properties of new materials. In this work, we propose a QSPR approach with the aim of estimating the α-relaxation dynamics of molecular glass-formers only based on their chemical structure. Firstly, we predict the T_g of the compound using a Fully Connected Network trained with a Simplified Molecular Input Line Entry System representation of the molecules. Then, we use the predicted value of the T_g as the input value for the Elastic Collective Non-linear Langevin Equation, which outputs the estimated α-relaxation dynamics of the compound. Finally, we validate our method by comparing the predicted results with experimental BDS measurements. We believe that this approach is a powerful tool in the design of new materials, as it allows not only to predict a physical property, but also to estimate a meaningful sector of the relaxation map even before the synthesis of a new material, saving financial and time resources.