Popular science summary

In order to produce everyday items from shoes to phones to toothpaste, many chemical processes are involved to make its ingredients, plastics and other components. Many of these processes take place in "solvents", liquids that facilitate the formation of these components in the right type and form to be useful. There are many of these solvents in use and they have a variety of properties in order to be able to produce the plethora of materials required in modern items.

But many of these solvents can be harmful for humans and the environment, evaporate easily or are flammable, posing risks that need to be carefully managed when using them. They are also commonly sourced from fossil fuels and can contribute negatively to climate change. It is one goal in science to find better and less harmful ways to produce things, and over the years some of the most harmful solvents have been retired and substituted.

In this thesis we investigate a group of new modern solvents, called "Deep eutectic solvents" (from here DES). They can be made by simply mixing two or more common ingredients at room temperature or under moderate heating. One of their strong points is that these ingredients can be things like sugars and other materials already produced on a large scale for from bio-sources, making them potentially more sustainable and less environmentally harmful. Another pro is that due to the many components available, and the change in solvent properties with components, component ratios and additives, they have a good potential as "designer solvents" with tailorable properties due for specific applications. There have been a range of applications found for them, but as they still have limits in predictable interactions and relatively high viscosity, research in this field is very active.

One of the main concepts behind DES is the eutectic – a property describing the phenomenon of a reduced melting point when mixing two components, relative to the melting points of each component. A famous example of this in DES is the mixture of urea and choline chloride, both molecules that can be found in the body, which in their pure form are solids, looking similar to sugar, but turn into a liquid upon mixing at a specific ratio even without heating. These liquids can then be used as solvents at room temperatures.

These DES have been found to have many unique properties, which help them be able to dissolve, assemble or react materials in them in interesting ways. Here we looked at the structure and interactions of some of these DES systems. Knowing how the molecules and even their atoms interact in these liquids can help understand how these DES form and interact with other molecules. This can help both the basic understanding, and hopefully future predictions, as well as laying the foundation for further application tests.