U.S. DEPARTMENT OF ENERGY

NATIONAL ENERGY TECHNOLOGY LABORATORY

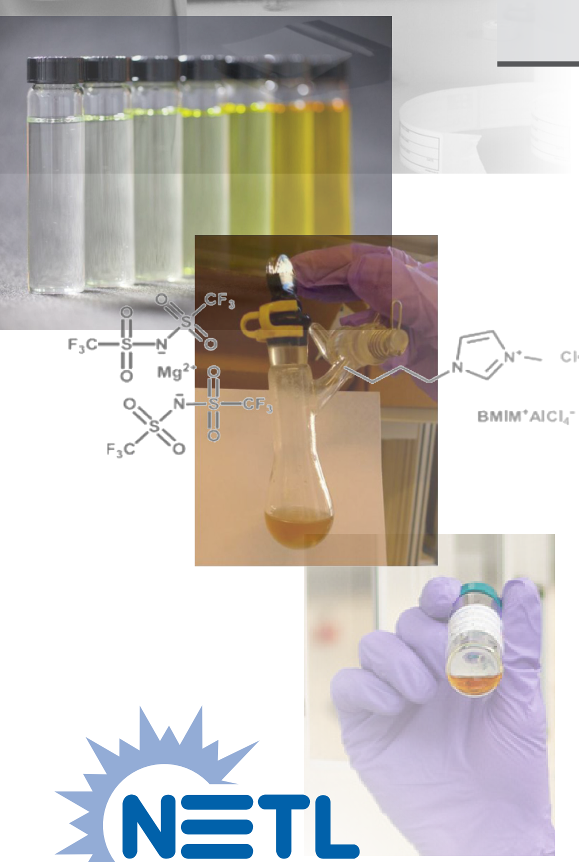
NETL is a U.S. Department of Energy national laboratory that produces technological solutions to America's energy challenges. For more than 100 years, the laboratory has focused on developing tools and processes to provide clean, reliable, and affordable energy to the American people. Three NETL research sites—Albany, Ore., Morgantown, W.Va., and Pittsburgh, Pa.—conduct a broad range of energy and environmental research and development activities that support DOE's mission to advance the national, economic, and energy security of the United States.

Technology transfer and commercialization lie at the heart of the National Energy Technology Laboratory's (NETL) mission, directly addressing U.S. energy research and development needs. NETL is committed to uphold America's trust through wise investment of U.S. taxpayer dollars. With this funding, we support technology innovation that private companies take to market to improve the cost, reliability, and environmental impact of our Nation's energy production and use. Spin-off technologies are also commercialized by the private sector to spur economic development and support national security.

Our partnerships are conducted in ways that ensure fairness of opportunity, promote U.S. economic interests, protect national security, support small and start-up businesses, and allow for competition within the private sector. Innovations emerging from NETL's programs are taking root and finding commercial success.

Ionic liquids:

A materials platform for technology development



Ionic Liquids: Solvent for the Future

Technology development has widened in scope over the past decade to include not only creating better products but also considering sustainability. As this shift has occurred, ionic liquids (ILs) have received greater interest for a wide variety of applications. Ionic liquids are nonvolatile salts, which are liquid under ambient conditions and can often diminish or alleviate environmental concerns by eliminating volatile organic compound emissions and taking the place of more hazardous materials. Perhaps the most important characteristic of ILs is their incredible variety. It has been estimated that there are 10^{18} ILs that could be created based on known chemistry. This nearly infinite ability to alter the structure of the materials leads to a similar and much more important opportunity to tailor their properties to specific applications.

Ionic liquids are being considered for an amazingly diverse set of applications including batteries, processing of polymers and cellulose, and polymer additives. Commercial interest in ILs is high with dozens of companies starting "green" materials development projects based around them. The first and best known example of a commercially successful IL-based operation was the BASIL™ process implemented by BASF to improve the efficiency of chemical synthesis. Several other concerns including Eastman Chemical and Petrochina have now begun operation of major processes using ILs as well.

The National Energy Technology Laboratory-Regional University Alliance (NETL-RUA) has spent the last 7 years developing the tools and expertise necessary to create new ILs with specifically targeted properties for CO_2 capture. The NETL-RUA Integrated Technology Development approach revolves around combining multiple

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research disciplines in a highly focused problem-solving methodology (Figure 2). The collaborative partnership between NETL and the five major regional universities of the NETL-RUA grants access to a vast array of expertise and facilities for the implementation of this methodology. These resources are now available to address the host of applications for which ILs are being considered.

> *"The most fundamental and lasting objective of synthesis is not production of new compounds, but production of properties."*
>
> George S. Hammond, Norris Award 1968

Properties of Ionic Liquids

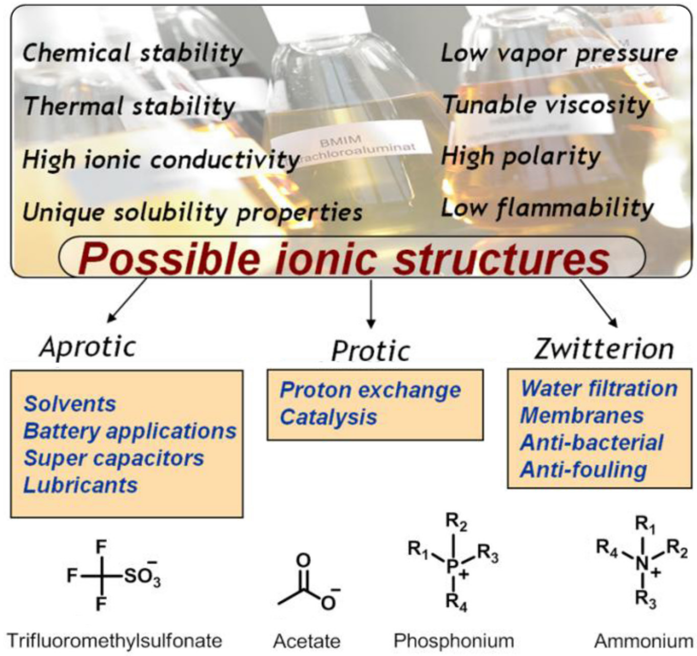

Figure 1: Ionic liquids are diverse, liquid salts with a variety of useful properties.

Integrated Technology Development

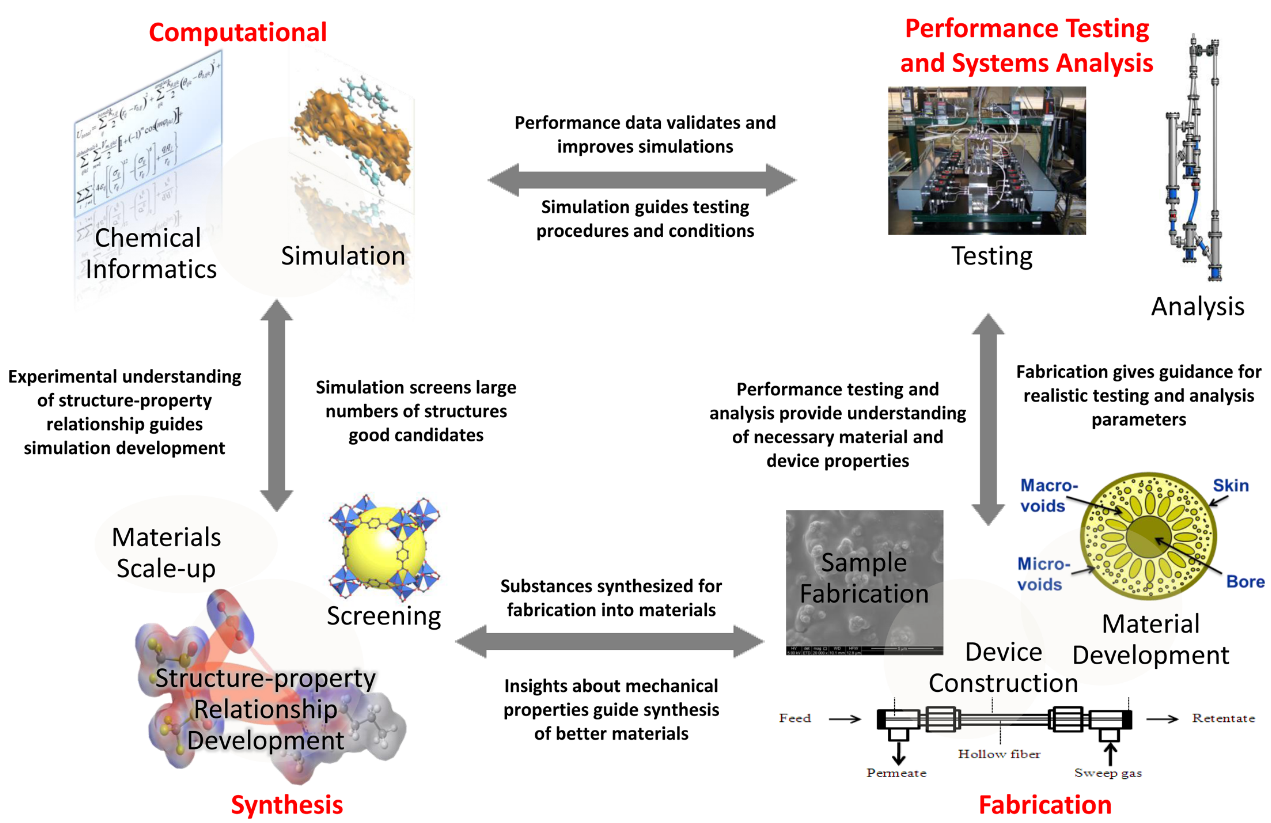

Figure 2: The NETL-RUA Integrated Technology Development approach.

Ionic Liquids-Based Research Areas

Structure Property Relationships of Ionic Liquids

Selecting ILs with the appropriate attributes for an application is a difficult task due to the effectively infinite number of possible structures. NETL-RUA researchers have collaborated with UC-Berkeley scientists to develop methodologies for mapping properties of ILs via computational and information science. The resulting property map (Figure 3) for a given class of ILs allows for physical properties, such as viscosity, solubility, and self-diffusivity, to be predicted and candidate ILs to be selected with the ideal values for each. This screening tool narrows the pool of candidate compounds to a few materials of interest, which can then be synthesized, characterized, and tested. This rapid screening of a huge library of structures results in materials that better match specifications and have an improved chance of success in a given application.

The NETL-RUA has used the property map shown in Figure 3 to screen 350,000 ILs for properties critical in carbon capture. The data show that the choices of the cation and its substituents as well as the anion can enhance or suppress the properties of the ILs for this application. Figure 4 shows an example of how information gleaned from this sort of analysis was used to locate ILs that are stable at temperatures of interest for pre-combustion carbon capture.

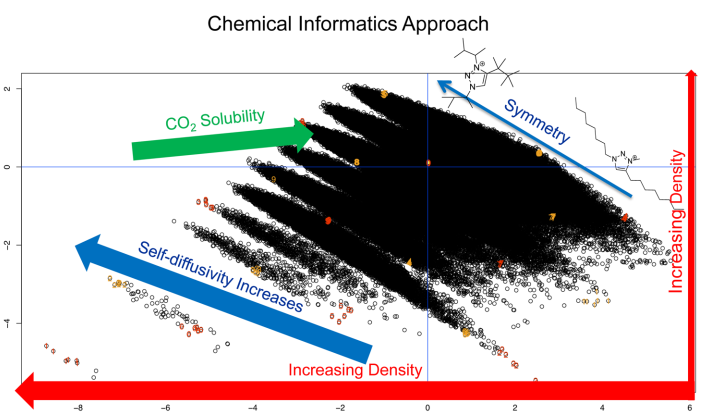

Figure 3: Property map for 350,000 ILs giving insight into the effect of density on CO_2 solubility, viscosity, and self diffusivity.

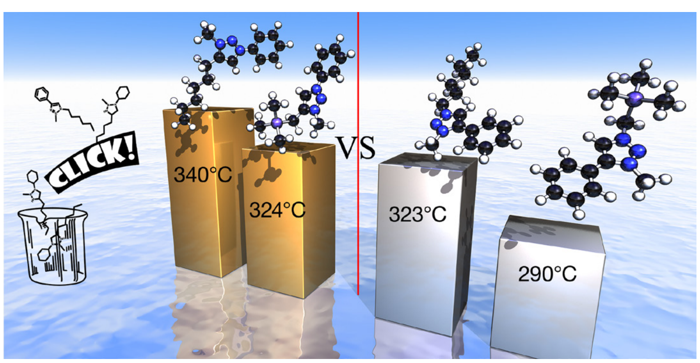

Figure 4: The effect of molecular structure on decomposition temperature for triazolium ILs synthesized using NETL's proprietary click chemistry.

Ionic Liquids in Membranes

The knowledge gained from the structure-property relationship studies undertaken to develop CO_2 solvents has also allowed the NETL-RUA to explore the next generation of gas separation devices, membranes. Membranes have the advantages of relatively simple process control and favorable energetics, but these advantages come at the cost of increased demands on materials. Using Integrated Technology Development and the resources of the NETL-RUA, researchers were able to produce the first IL-based facilitated transport membranes and demonstrate that their performance was superior to any similar membranes yet developed for separating CO_2 from H_2.

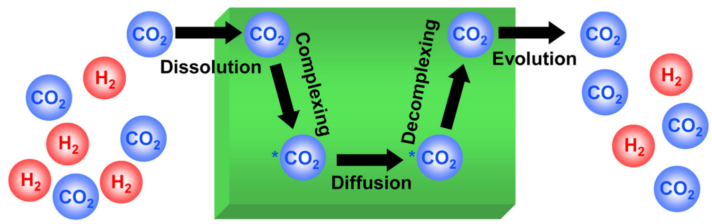

Figure 5: IL Ionic liquids-based facilitated transport membrane for separating CO_2 from H_2 for pre-combustion capture.

Processing of Cellulose

Processing and purification of cellulose in ILs is another area of research interest that has been examined in collaboration with Professor Sixta from Aalto University (Finland).

Ionic liquids are effective solvents for cellulose, but traditional ILs tend to decompose and suffer increases in viscosity under the process conditions. The collaborative project is aimed at developing cost-effective alternatives to these ILs with better performance using complementary computational and experimental techniques.

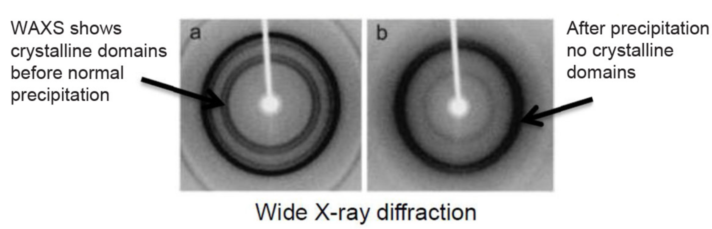

Figure 6: Wide angle X-ray spectroscopy showing the relative crystallinity of cellulose samples before and after dissolution in a novel ionic liquid.

Metal Deposition

The ionic nature of ILs makes them ideal candidates for electrochemical applications including deposition of metals. The NETL-RUA has evaluated ILs for magnesium battery applications because of their exceptionally high potential window, which may be useful in a variety of other electrochemical applications as well. Researchers have, for example, developed ILs which show promise in deposition of aluminum. These materials were specially developed for the deposition of aluminum on iron, and care was taken to improve the wetability of the metal surface resulting in smoother coatings than are possible with other processes (Figure 7).

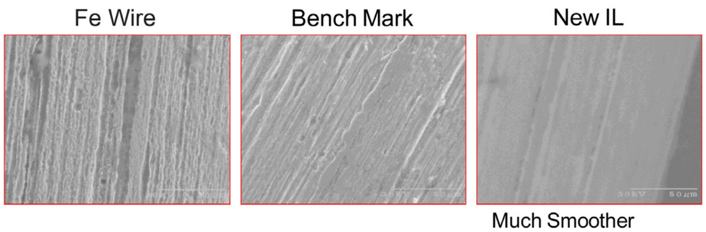

Figure 7: Deposition of aluminum using ILs.

Lubricants and Thermal Fluids

The high heat capacities and thermal stability of ILs make them excellent candidate materials for heat removal and lubrication applications. The materials are already used commercially as vacuum pump lubricants because of their lack of vapor pressure and overall chemical stability. NETL-RUA researchers have developed ILs with these purposes in mind and helped a local company to use the new materials as lubricants for pumps in a geothermal application.

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