R & D facts

U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

Carbon Sequestration

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Molecular Design of CO_2 Ligands Ionic Liquids and Poly (ionic liquids)

Justification and Background

The potential for various ionic liquids (ILs) and poly(ionic liquids) (PILs) to capture CO_2 is being investigated. Papers published by Radosz and co-workers indicate that PILs can have very larger CO_2 uptake compared with ILs. One of their most surprising results was that four of the IL monomers they tested had essentially zero uptake capacity for CO_2, whereas when polymerized, the corresponding PILs showed very large uptake at a temperature of 22 °C and a pressure of about 0.8 bar. Molecular modeling combined with COSMOtherm is being used to gain insights into these surprising findings

Approach

Turbomole ab initio calculations have been used to predict the σ profiles for the following PIL/IL pairs: PVBIH/VBIH, PVBIT/VBIT, PBIMT/BIMT, PVBTMA/VBTMA, PMATMA/MATMA, PVBBI/VBBI and on the [bmim][BF4] and other ionic liquids. In cooperation with an industrial researcher, COSMOtherm calculations using the σ profiles have been used to estimate the Henry's law constants and solubilities for CO_2 in the ILs and PILs at the experimental condition of 22 °C and 0.8 bar. Results from these calculations are summarized in Table 1. Good agreement for some of the PILs and ILs tested have been found but there are discrepancies for several systems. Therefore an experimental program has been initiated to confirm the computational results.

Table 1. Experimental and calculated CO_2 solubilities for various poly(ionic liquid)s.

Poly(ionic liquid)s	Experiments	Calculations
PVBTMA+BF_4	10.2	2.2
PMATMA+BF_4	8.0	1.2
PVBIH+PF_6	2.7	3.3
PVBBI+Tf_2N	2.2	3.1
VBBI+Tf_2N	N/A	3.0
PVBIT+BF_4	2.2	2.7
PBIMT+BF_4	1.8	1.9
BIMT+BF_4	1.3	1.8
bmim+BF_4	1.3	1.7
VBIH+PF_6	0.0	3.1
VBIT+BF_4	0.0	2.5
VBTMA+BF_4	0.0	0.7
MATMA+BF_4	0.0	1.0

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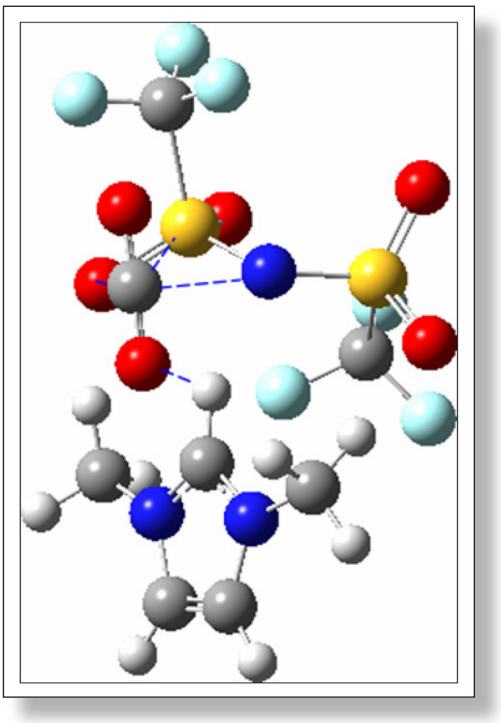
Project Goal

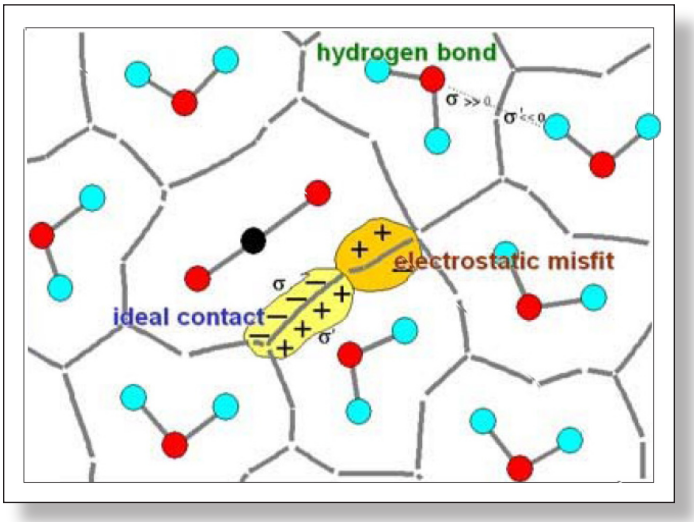
Develop ionic liquids or poly (ionic liquids) to be used as sorbents or membranes which will allow a decrease in the cost of carbon dioxide capture from coal-based power generation to such extent that 90 percent of the carbon dioxide produced may be captured, transported and sequestered at less than a 10 percent increase in the cost of the energy services.

Expected Benefits

Development of an ionic liquid/poly (ionic liquid) model capable of accurately predicting material properties will guide the application of these ionic liquid based materials to membrane and sorbent development for CO_2 capture.



CO_2 binding with the anion (Tf2N)



COSMO-RS is a theory that describes the interactions in a fluid as local contact interactions of molecular surfaces. The interaction energies are quantified by the values of the two screening charge densities σ and σ' which form a molecular contact.