

PNNL- 35284

# Development of Transformational Solvents for CO<sub>2</sub> Separations - CRADA 363 (Abstract)

CRADA 363 (PNNL 65872)

February 2024

*David J Heldebrant*

GE Global Research

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the U.S. Department of Energy  
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## Abstract

The primary objective of this CRADA activity is to use a combined molecular modeling and experimental validation approach to refine and develop transformational solvents for carbon capture. PNNL's role on this project is currently funded by the Department of Energy's (DOE) Office of Fossil Energy (OFE). PNNL is developing advanced molecular modeling based on their CO2BOLs solvent platform as a demonstration solvent for the activity; the model was developed and compared against measured data for CO2BOL derivatives. Here, a CRADA with PNNL and GE will leverage their current molecular models and apply them to solvent classes that operate on carbamate chemistry, specifically GE's aminosilicone solvent class. The molecular models will be used to predict physical and thermodynamic properties, such as viscosity, as a means to predict advanced formulations with reduced viscosity compared to current aminosilicone derivatives, enabling optimized thermodynamic and kinetic metrics for economical carbon capture for this class of materials. Together, PNNL and GE will develop a comprehensive means of linking molecular modeling parameters to intermediate physical properties as a means to improve solvent performance.

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