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Molecular simulations turn ‘green’: An integrated approach to accelerate the development of CO₂ capture solvents

Vassiliki-Alexandra Glezakou

Pacific Northwest National Laboratory, USA

The ever-increasing carbon footprint from post-combustion large point sources has made greenhouse emissions one of the most urgent environmental problems commanding immediate attention. Solvent technologies for CO₂ capture have become some of the most promising solutions, with aqueous amines being the industrial benchmark system. However, their high regeneration costs render them prohibitive for many of the flue gas applications. The U. S. Department of Energy has invested in the development of different classes of solvents in an effort to reduce parasitic loads and fully deploy these technologies by 2030. In the present talk, synchronized computational, experimental and engineering efforts directed towards the deliberate design of single-molecule, CO₂-binding organic liquids will be described. The PNNL developed CO₂ capture technology are an attractive alternative to amine-based solvents, but they are plagued by high viscosities at high CO₂ loadings. Using state-of-the-art computational methods and large models we describe the key structure parameters that allowed us to create reduced models for fast screening of potential candidates with low viscosity. Additionally, *ab initio* molecular dynamics and enhanced sampling methods made possible the computation of reaction free energetics for CO₂ binding and proton transfer that control important acid/base equilibrium. Consequently, we were able to make tangible hypotheses towards synthetic targets with appreciable viscosity reductions especially at high CO₂ loadings. These efforts have led to a fundamental understanding of the underlying factors controlling viscosity and the development of several classes of green solvents.

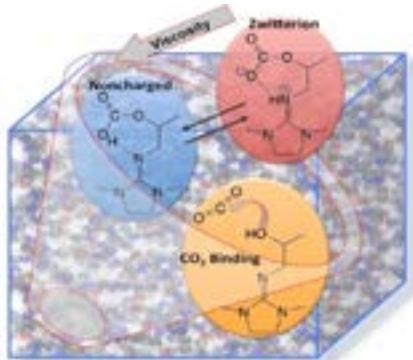


Figure1: Molecular simulation has enabled the discovery of new chemistries resulting in a significant reduction of viscosity in CO₂ capture solvents.

Biography

Vassiliki-Alexandra Glezakou is a Senior Scientist at Pacific Northwest National Laboratory with 20+ years of experience in theoretical/computational methods and simulations techniques. Her research aims towards the understanding, prediction and control of materials relevant to new technologies. Current interests include transition metal chemistry with applications in catalysis and hierarchical materials, materials development for radionuclide remediation, design of CO₂ capture and transformation solvents and development of reduced order models to accelerate materials discovery.

Vanda.Glezakou@pnnl.gov

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