

4<sup>th</sup> International Conference on

# PHYSICAL AND THEORETICAL CHEMISTRY

September 18-19, 2017 Dublin, Ireland

## Molecular design strategies for task-specific solvent technologies

**Vassiliki-Alexandra Glezakou**

Pacific Northwest National Laboratory, USA

CO<sub>2</sub> capture from power plant exhaust is a complex problem that requires the capture and removal of massive quantities of gases. Solvent technologies for CO<sub>2</sub> capture and conversion have become one of the most promising solutions with aqueous amines being one of the industrial standards. However, their high regeneration costs render them prohibitive for many of the large-scale applications in power generation. My presentation will outline the computational approach used toward the deliberate design of single-molecule CO<sub>2</sub>-binding transformational solvents. These types of solvents constitute an attractive alternative to the water-based solvents, but are hampered by exponentially increasing viscosities at high CO<sub>2</sub> saturation. Using state-of-the-art computational methods, like enhanced sampling methods for reaction free energetics in explicit solvent models using *ab initio* molecular dynamics, we describe the key structural parameters that allowed us to create reduced models for fast screening of solvent libraries. This approach led to tangible hypotheses as to the synthetic protocols that have already identified candidate molecules with appreciable viscosity reductions at target loading levels.



**Figure 1:** Schematic representation of concerted design efforts to accelerate solvent design for CO<sub>2</sub> capture.

### Biography

Vassiliki-Alexandra Glezakou is a Computational Chemist with over 20 years of experience in atomistic simulations, with particular emphasis in transition metals chemistry and condensed phase systems relevant to carbon capture and conversion, catalysis and materials properties. Her focus of recent research is on the structure, vibrational spectroscopy and structure/activity correlations in a diverse ensemble of problems such as catalytic activity of metal clusters and oxide supports, transformative solvents for post-combustion carbon dioxide separations, mechanistic studies of MOF nucleation.

Vanda.Glezakou@pnnl.gov

### Notes: