Multiscale simulation of Amino-acid ionic liquids (AAILs): Properties and CO_2 Capture Mechanism

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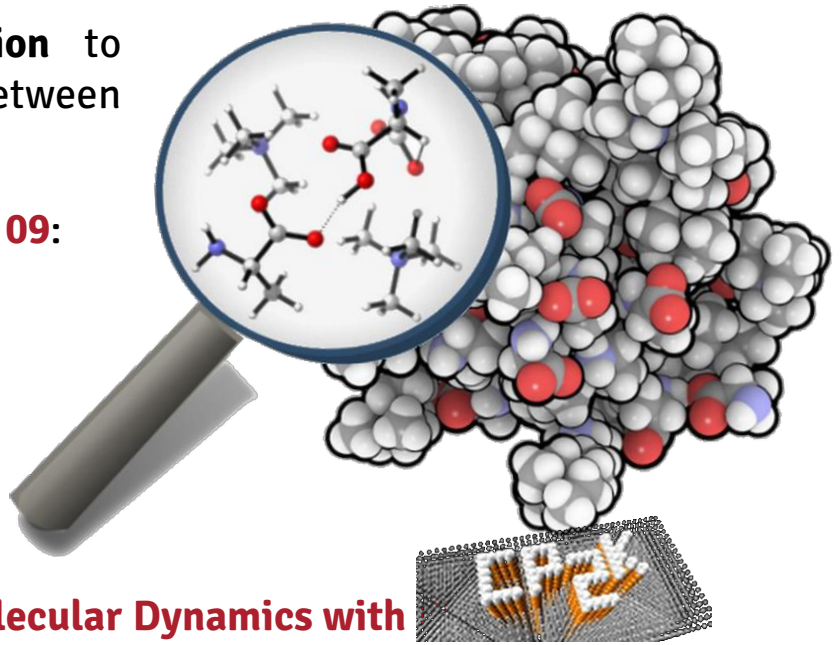
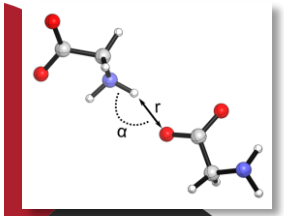
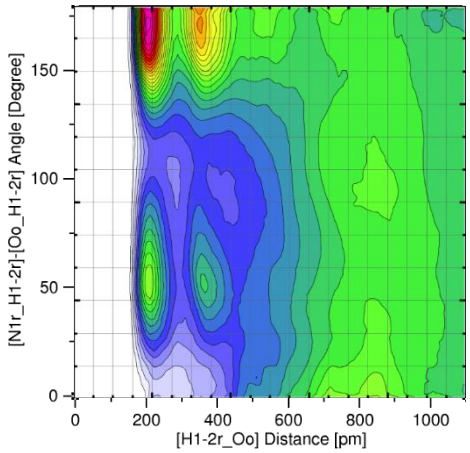
- Aim: Exploring the **mechanism of CO_2 absorption** to understand the different capacity observed between different AAILS (1:2 or 1:1).

➢ Exploration of three different pathways with **Gaussian 09**:
Model: 2 ionic pairs $[N_{1111}]^+[\text{L-alanine}]^-$
✓ 1:1 Mechanism: formation of a carbamate

❑ How to explain the discrepancy with the 1:2 capacity observed? Dimerization of the carbamate?







➢ **An-Initio Molecular Dynamics with**

- Two models: $[N_{2222}]^+[\text{L-ALA}]^-$ and $[N_{2222}]^+[\text{GLY}]^-$
- Created low density cell with 35 Ionic Pairs (>1000 atoms). Built with Packmol / AMBER (gaff)
- CP2K:
  1. NPT until density equilibrated.
  2. NVT trajectory 100ps.
  - Analysis with Travis

➢ **Next step: adaptive QM/MM to go larger and longer!**