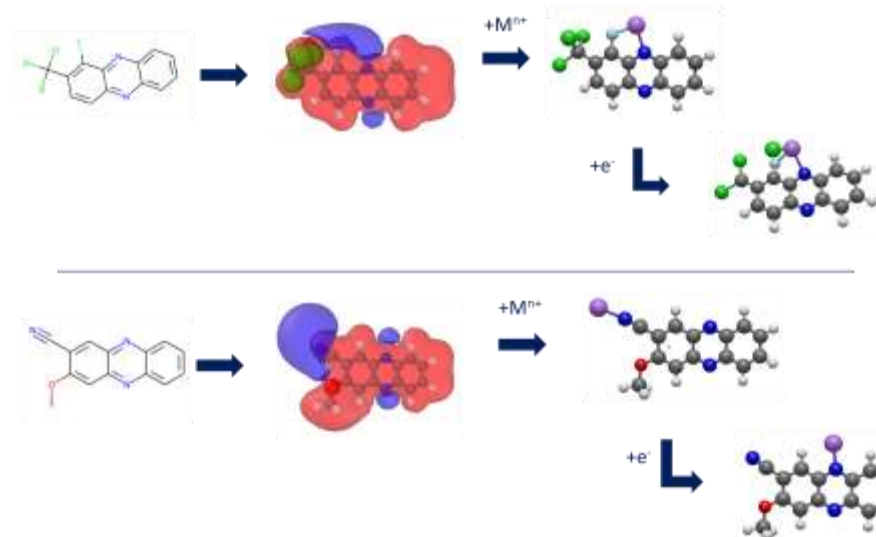
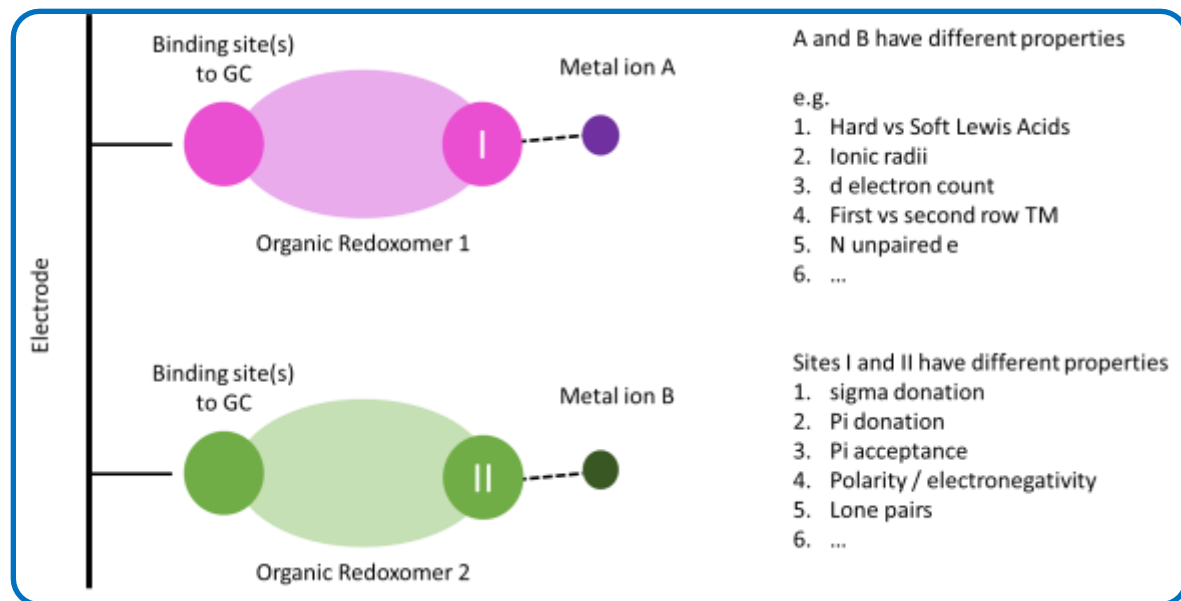


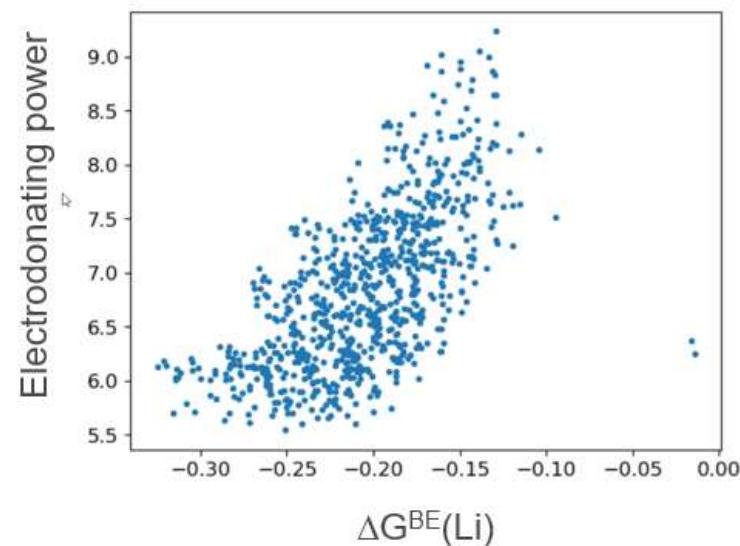
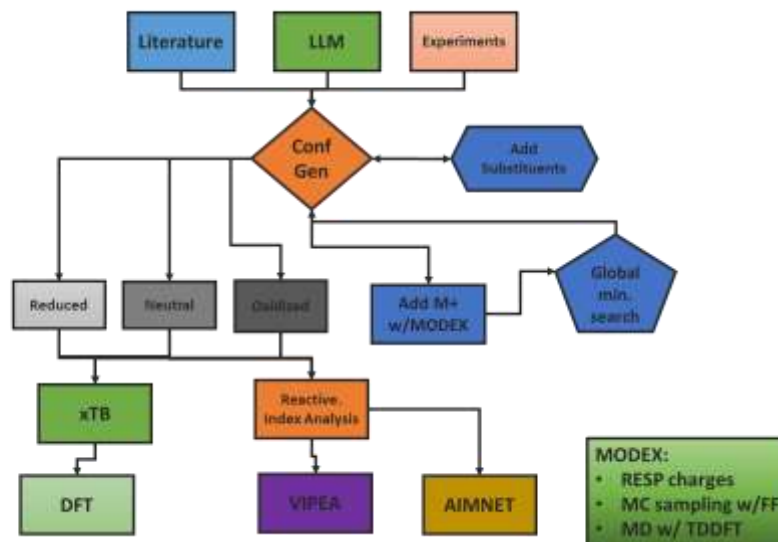
AI ASSISTED MOLECULAR DESIGN OF REDOXMERS FOR METAL ION RECOVERY IN WATER



WORKFLOW

Mangowf

- Fireworks
- Orca
- xTB
- ASE
- Amber
- Rdkit
- AIMnet (torch)



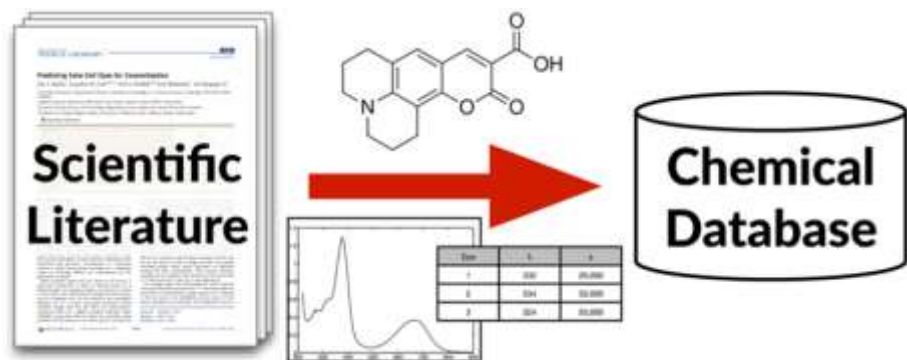
Contact:

cps.chemmat@anl.gov

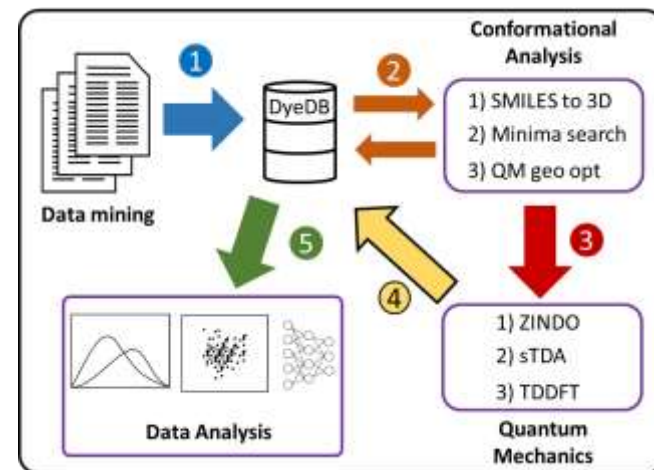
#cps_chemmat @cels slack

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AUTOGENERATED DATASETS AND ONLINE LEARNING TO ACCELERATE AUTONOMOUS DISCOVERY



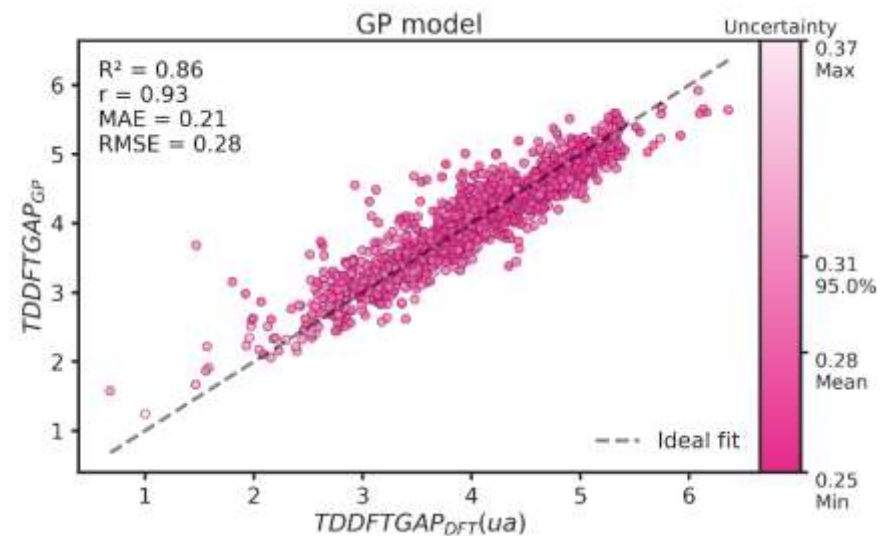
DATAMINING



HPC WORKFLOWS



GENERATIVE AI



PREDICTIVE AND EXPLAINABLE AI MODELS

Contact:

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