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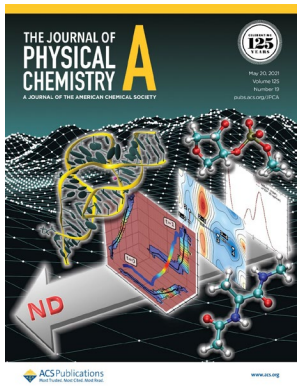

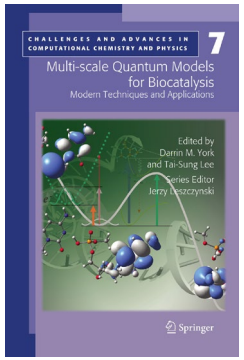

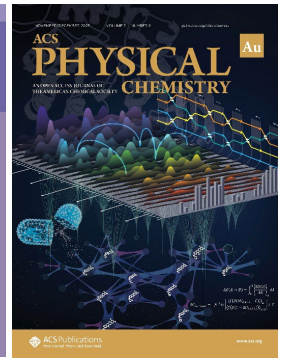

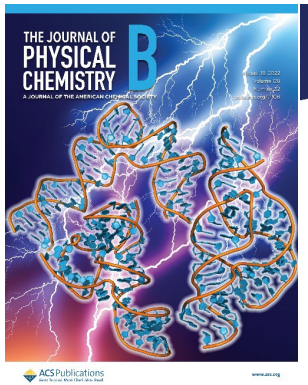

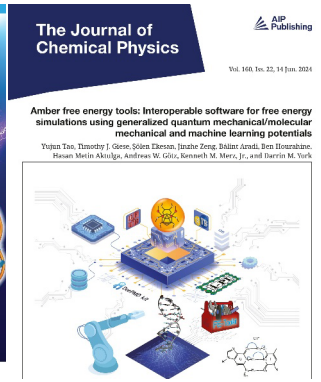

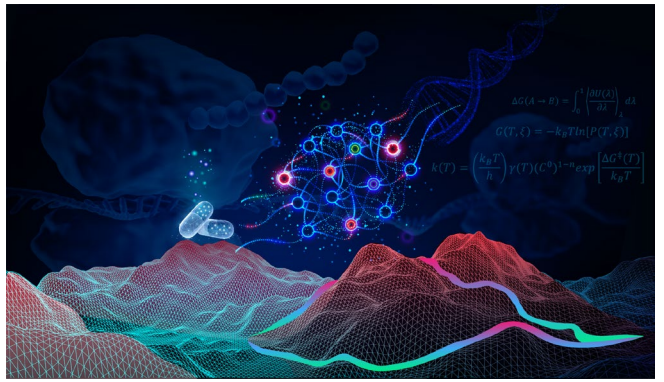

Advancing AI tools for drug discovery and enzyme design

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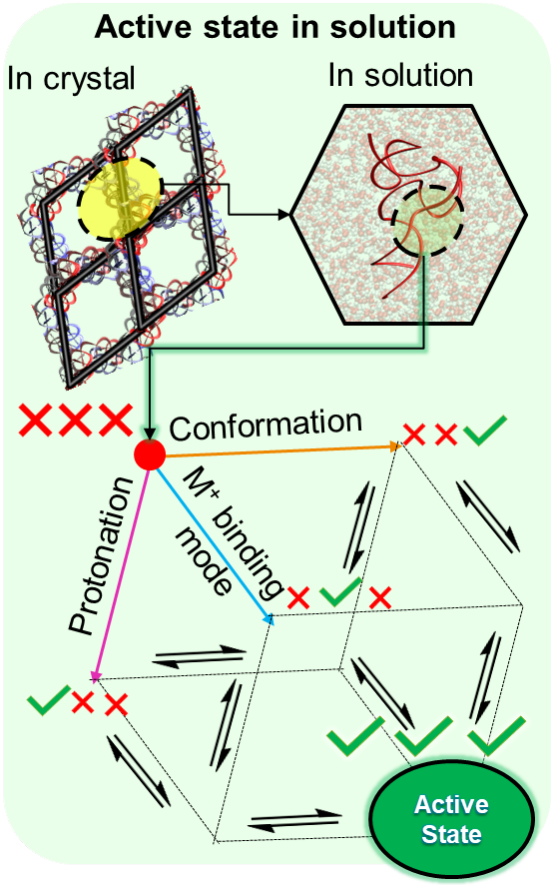
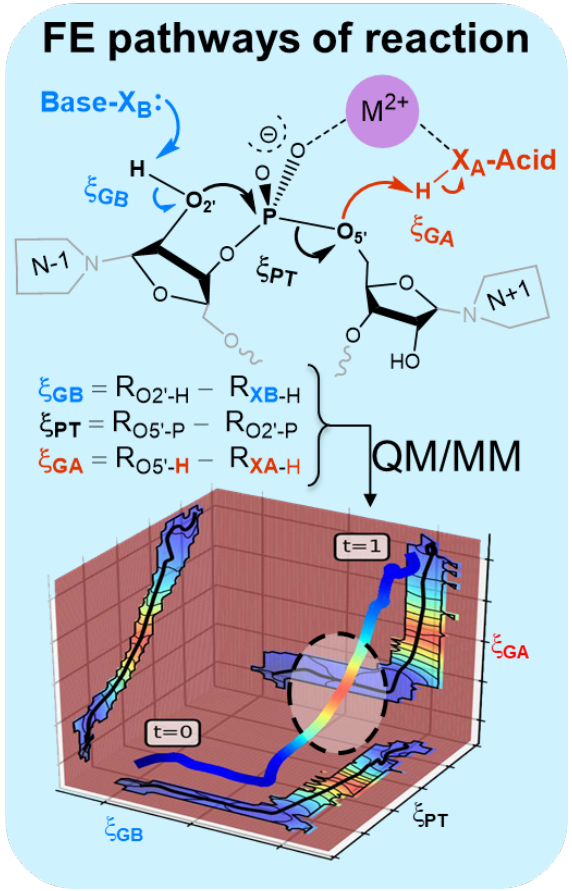
Enzyme Design





MM FF

↓

se-QM 10^3X

MLP
10-10^3X

↓

***ai*-QM 10^6X**

↓

hc-QM

AI/DS Opportunities

- Prediction of the "active state"
- QM/ML-potential for catalysis
- ML prediction of minimum free energy paths in collective variables

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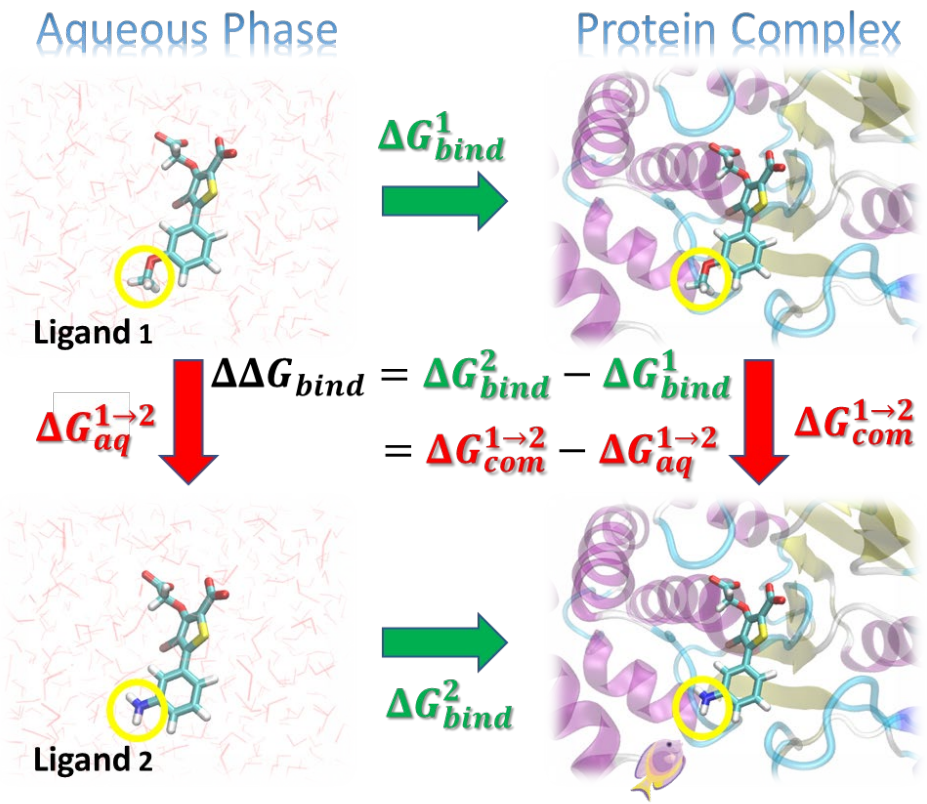
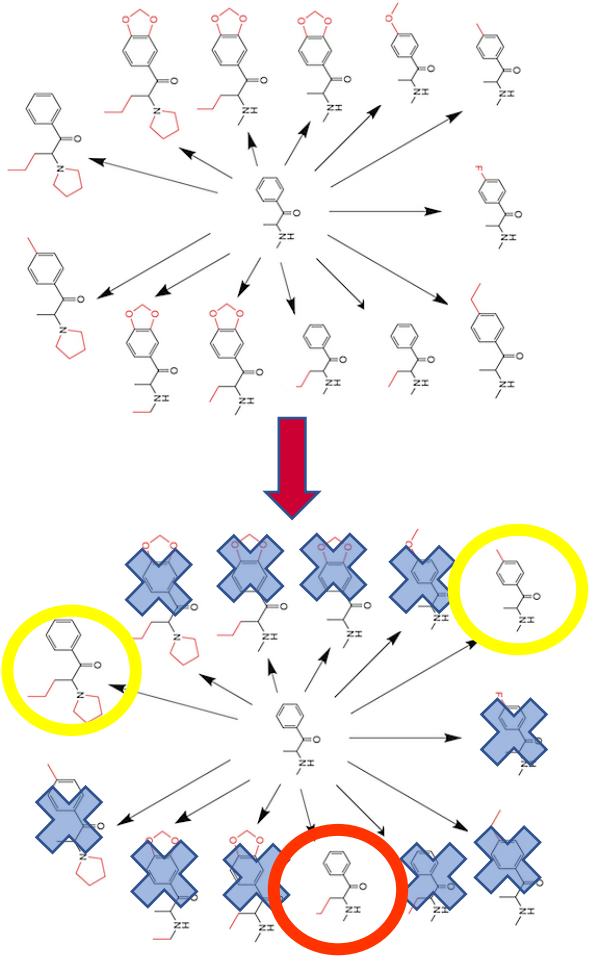
Drug Discovery





AI/DS Opportunities

- Protein variant structure prediction
- Ligand docking prediction
- ML-potential for drug-like molecules (tautomers/protonation states)
- AI-FEP for large-scale target-specific screening
- Fast new models for ΔG_{bind} prediction

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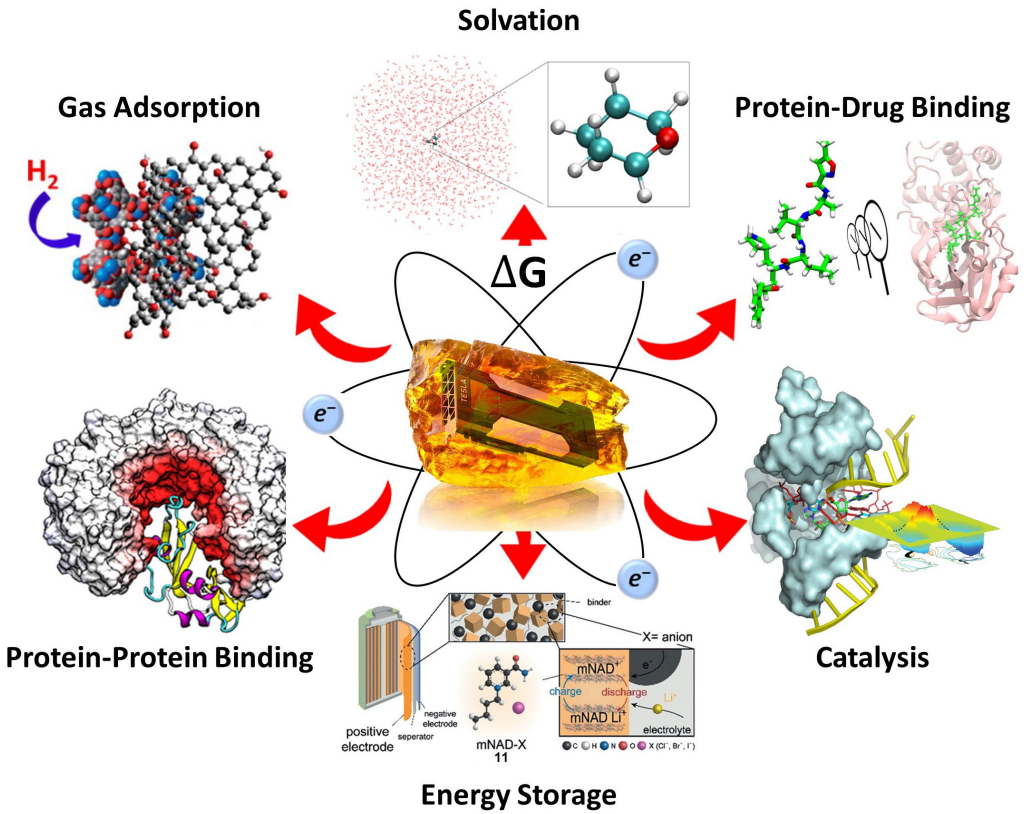
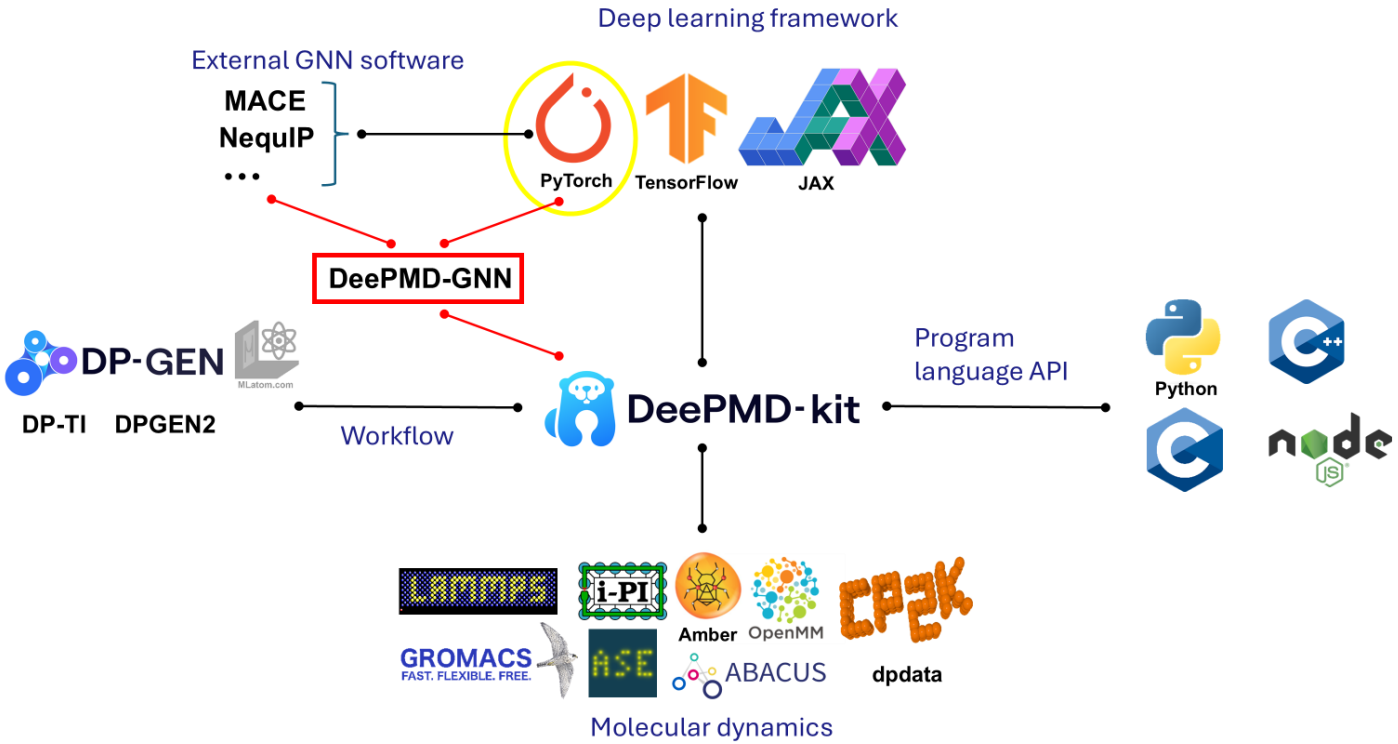


AMBER Molecular Simulation Software Suite



DeePMD-kit software for deep learning-based interatomic potential energy models

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