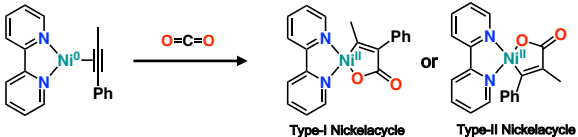


Ni-Mediated Regioselective CO₂ Insertion into Coordinated Alkynes



High-Performance Computing (HPC)



AutoMech



Aurora

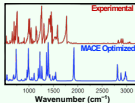


ΔG_{rxn} , $\Delta\Delta G$

Architector
(MACE-large)

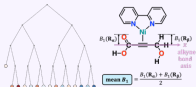
Generate optimized structures and thermochemical energy datasets

Experimental Validation (EV)



Validate computed structures with IR spectra and regioselectivity

Machine Learning (ML)



Identify descriptors controlling reactivity and regioselectivity