

# Electrochemical interactions in bimetallic molybdenum nitrosyl complexes incorporating $\mu$ -oxo bridges – DFT modeling



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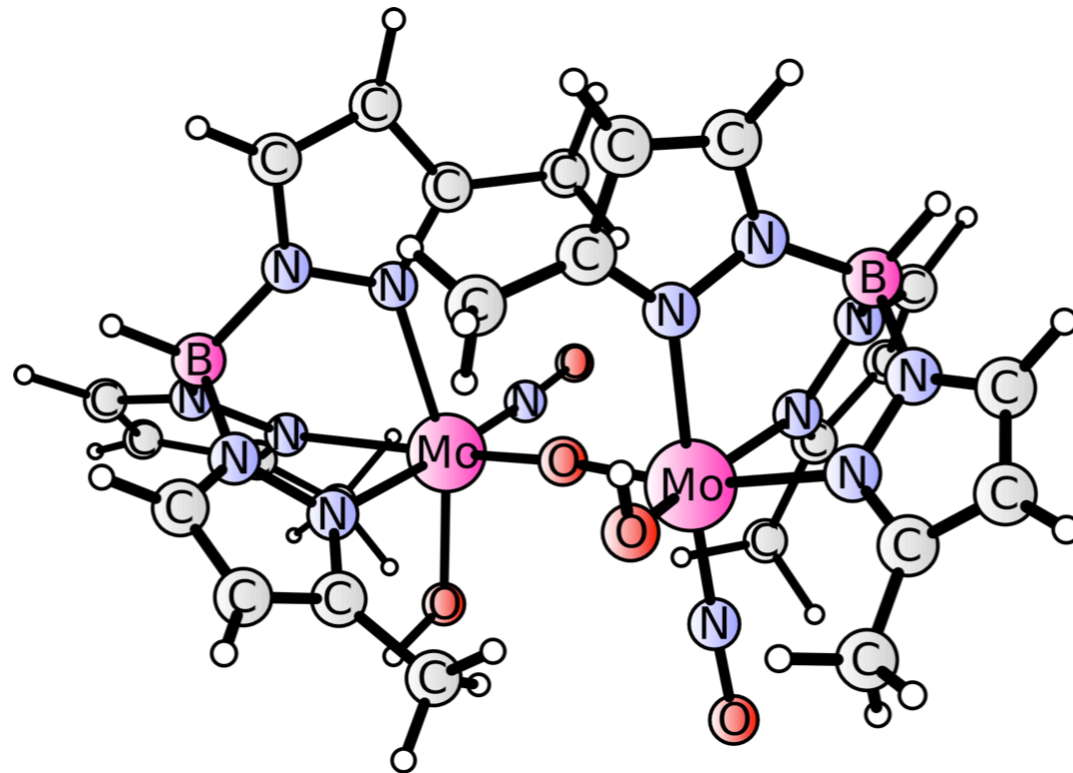
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## Purpose

Study of electronic structure of mixed-valence species

- unpaired electron delocalization

**Mixed valence compounds** - molecules with two (or more) redox-active metal centers connected *via* appropriate bridging ligand



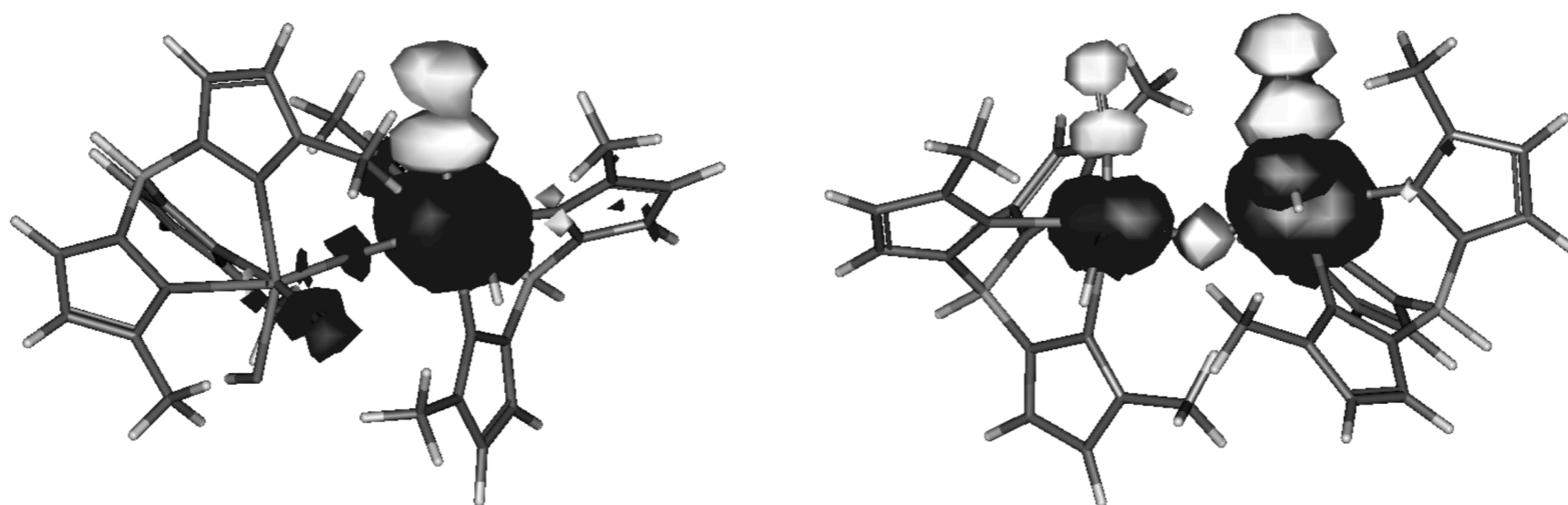
**Large molecules** (around 100 atoms) - significant computational cost



**Density Functional Theory**

### Detailed analysis:

- geometries
- redox potentials
- IR spectra
- spin densities



*Spin density of mixed-valence species*

Calculations have shown:

- nonequivalence of Mo centers is energetically favorable
- the unpaired electron is localized on one of the molybdenum centers with partial delocalization in twisted compound