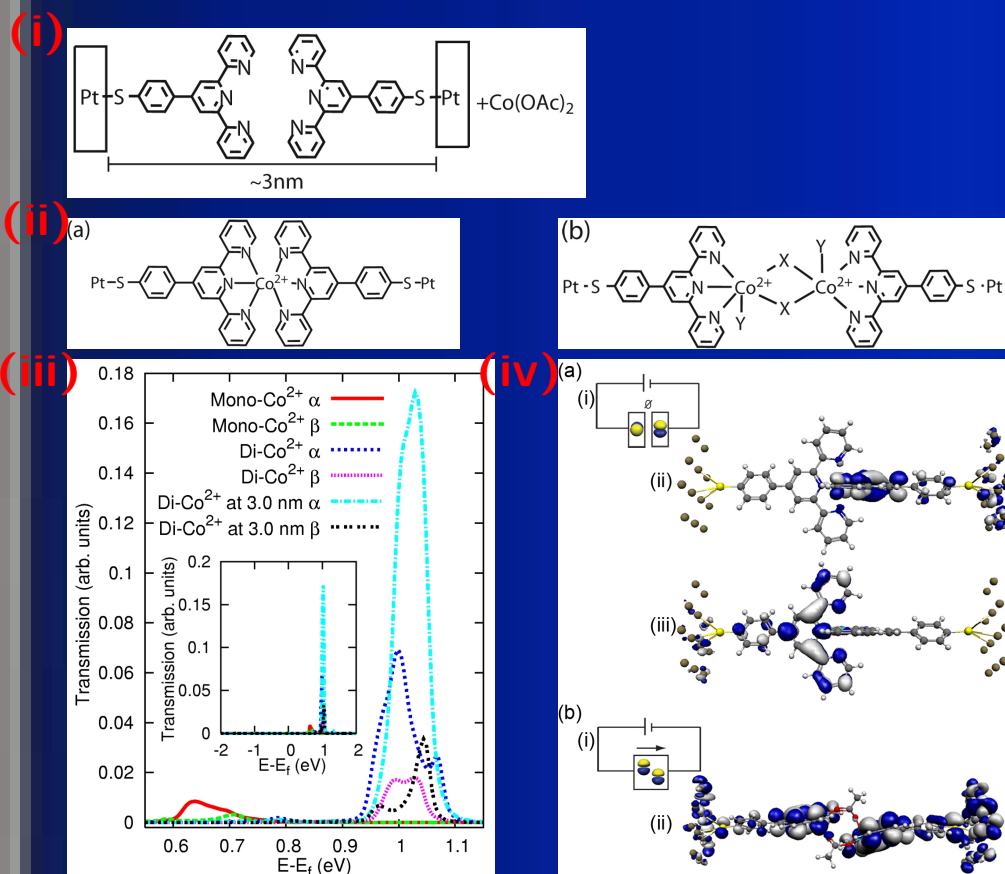


Molecular Conductance: Modeling physical and chemical control

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An experiment demonstrating molecular conductance involving a molecularly functionalized gap by thiolated terpyridine SAMs, which becomes conductive ONLY upon introducing Co(II) acetate [Tang et al, *ang. chem.*, 2007, 46, p3892] is computationally analyzed[†]:



Confinement-induced π -stacking interactions, which are mediated by acetate ions and cobalt complexation, enable the observed conductances.

[†]Perrine and Dunietz, *J. Phys. Chem. A*, 2008, 112, p2043.]