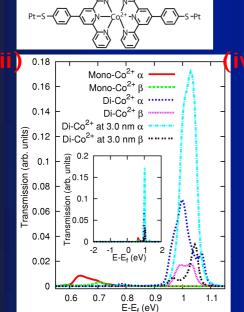
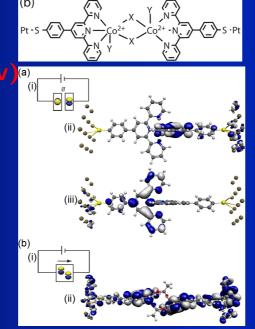
## Molecular Conductance: Modeling physical and chemical control

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

Pt S N N +Co(OAc)<sub>2</sub>





(i) Fabrication scheme of a Coterpyridine complex device. (ii) Molecular complex models with: (a) single Co(II) ion bridge and (b) di-Co(II) ions bridged by OAc. (iii) Corresponding transmission functions: the di-Co(II) complex dominates the transmission. (iv) Illustrating the effect of the  $\pi$  stacking interactions to result with a conductive electronic channel.

Confinement-induced  $\pi$ -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.]

