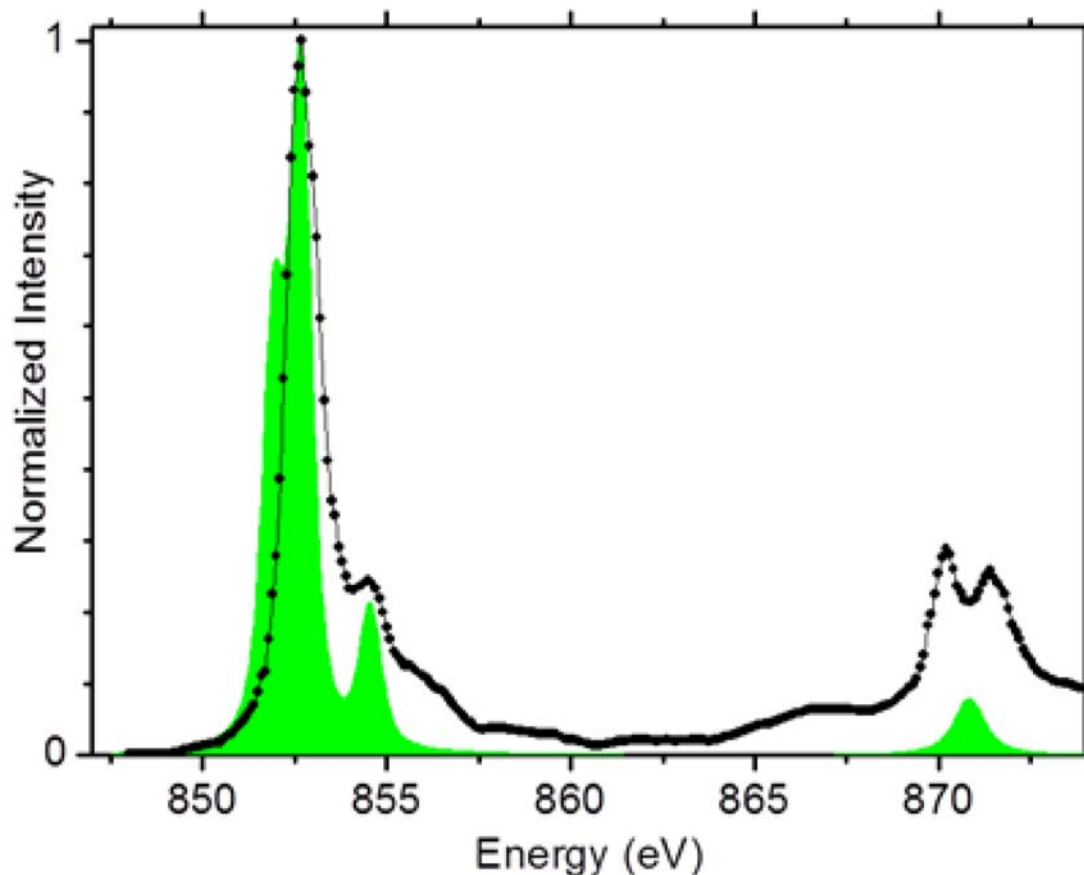


Charge transfer calculations multiplet spectrum of Ni²⁺



- Calculate the atomic multiplet spectrum of Ni²⁺. Set all parameters to zero.
- Set the 2p spin-orbit coupling to 1.0. Repeat the calculation. Explain the spectrum.
- Set the Slater integrals to 1.0. Repeat the calculation. Explain the spectrum.
- Set the 3d spin-orbit coupling to 1.0. Repeat the calculation. Explain the spectrum.
- Run a calculation using the following parameters: $\kappa = 0.9$, $10Dq(3d) = 0.7$ eV (*Crystal Field*), $\Delta(3d,Ld) = 4.3$ eV, $U(3d,3d) = 7.5$ eV, $U(2p,3d) = 8.5$ eV, $V_{eg}(3d,Ld) = 2.0$ eV, $V_{t2g}(3d,Ld) = 1.0$ eV (*3d-Ligands Hybridization*). How does the calculated spectrum compare with the measured spectrum of NiO?