Theory of Ni-2p3d3d resonant photoemission of Ni doped $SrTiO_3$

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$SrTiO_3$ has a band gap of 3.25 eV at room temperature, which would result in an absorption edge at UV wavelengths. Therefore, previous studies have suggested that the band gap can be reduced by doping Ni at the Ti position, shifting the absorption edge to the visible wavelength range. In a previous study [1], Ni was doped in $SrTiO_3$ thin films and resonant photoemission spectroscopy was performed on Ni in the thin films to study the electronic correlations of Ni.
My study aims to reproduce the resonant photoemission spectra as an initial step towards a better understanding of electronic correlations.

As a research method, the spectra obtained from multiplet calculations for a model with a ligand field added to the Ni single atom and the density of states of the clusters were used to reproduce the spectra for impurity Ni. The density of states of the clusters was calculated using VASP, a DFT-based ab initio calculation software, where, the Ti in one unit cell was replaced by Ni for a $2 \times 2 \times 2$ supercell, which was 12% doped as in previous studies.

The reproduction of spectra suggests that the strongest peaks of the resonance enhancement are due to electronic correlations originating from the Ni ligand field. This is similar to the result inferred by [1] and is considered to be a reasonable result.

References

[1] Fatima Alarab *et al*, Phys. Rev. B 104, 165129 (2021)