The development of ES2MS to spin polarization and ARPES calculations using multiple scattering theory for strongly correlated electron systems

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Multiple Scattering theory (MS) is one of the effective calculation methods for ARPES (Angle Resolved Photoelectron Spectroscopy). There are several methods for calculating the potential required for MS, but the methods and accuracy are controversial. Calculating better potential is important for improving the accuracy of ARPES calculations and understanding physical properties.

ES2MS (Electronic Structure code to Multiple Scattering code) [1] was developed as a package to calculate all-electron potential from VASP. It is included in the X-ray absorption calculation software FPMS developed by K. Hatada. This method is very powerful in that it can calculate potential from electronic states calculated by SCF using VASP with PAW. However, it was not possible to perform spin polarization calculation, and it was not adapted to magnetic materials.

We have implemented a new spin-polarized potential in ES2MS and successfully incorporated it into our one-step model Real Space Multiple Scattering theory (RSMS) [2].

Furthermore, we incorporated the on-site Coulomb repulsion effect (+U) and applied it to strongly correlated electron systems such as Fe_3O_4 and NiO.

Using this method, we directly calculated the surface potential of reconstructed Fe_3O_4(001) [3], which could not be reproduced using the LMTO. ARPES calculations using this potential successfully obtained patterns that could not be obtained using the conventional LMTO-bulk potential.

References

[1] J. Xu, C. R. Natoli, P. Krüger, …, K. Hatada computer physics communications **203** 331-338 (2016)

[2] P. Krüger *et al*, Phys. Rev. B **83**, 115437 (2011)

[3] M. Taskin, …, P. Krüger, *et al*, Phys. Rev. B **108**, 155403 (2023)