Multiband d-p model for the description of Sr_2RuO_4

K. Rościszewski[1] and A.M. Oleś[1,2]

[1] *Marian Smoluchowski Institute of Physics, Jagellonian University, Reymonta 4, PL-30-059 Kraków, Poland.*

[2] *Max-Plack Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*

We study electronic structure of multiband d-p model (similar to that used in ref. [1]) for the description of quasi-two-dimensional RuO_4 planes such as realized in Sr_2RuO_4. The model takes into account nearest neighbor anisotropic ruthenium-oxygen and oxygen-oxygen hoppings, intraatomic Coulomb interaction and Hund's exchange on both ruthenium and oxygens and additionally spin-orbit coupling on ruthenium.
We were motivated by an earlier abinitio cluster computations which reported charges on oxygen p-orbitals close to 5 and charges on ruthenium close to 6 instead of formal 6 and 4 (ref. [2]). The ruthenium eg orbitals were also found to be occupied [2] contrary to common believes, similarly like showed earlier for CoO_2 planes [3].

References:

[1] Sugimoto T, Ootsuki D and Mizokawa T 2013 *J. Phys. Soc. Jpn.* **82** 104
[2] Kaplan I G and Soullard J 2007 *Phys. Rev.* B **76** 174505
[3] Rościszewski K and Oleś A M 2013 *J. Phys.: Condensed Matt.* **25** 345601

This investigation was supported by Polish National Science Center under project No. 2012/04/A/ST3/00331