Electronic structure of skutterudite superconductors MPt_4Ge_{12} (M=Ba, Sr, La) – density functional calculations

J. Kaczkowski[1]

[1]Institute of Molecular Physics Polish Academy of Science, ul. M.Smoluchowskiego 17, 60-179 Poznan, Poland

Platinum germanides skutterudites (MPt_4Ge_{12}, M=Ba, Sr, La, Pr, Th) [1-9] are new type of superconductors with T_c less then 8.3 K. In this work the electronic structure of $SrPt_4Ge_{12}$, $BaPt_4Ge_{12}$ and $LaPt_4Ge_{12}$ within PAW method (VASP), ultrasoft pseudopotential (PWscf) and FP-LAPW (elk) method was calculated. The scalar relativistic approach and gradient approximation was used (PW91 and PBE). The influence of gold substitution on electronic properties of $SrPt_4Ge_{12}$, $BaPt_4Ge_{12}$ was also investigated (for experimental results for $BaPt_4Ge_{12}$ see ref. [5]). Density of states at the Fermi level [$N(E_f)$] was equal (from different methods): 8.25 for $LaPt_4Ge_{12}$, 8.6-9.1 for $BaPt_4Ge_{12}$ and 8.43-9.1 (all values in 1/eV*f.u. units) for $SrPt_4Ge_{12}$. From [1] this values are about 13 1/eV*f.u. for Ba and Sr, however in [5] in case of Ba the value was equal 8.8 1/eV*f.u. which is very close to present results. Gold substitution increase value of $N(E_f)$ from 8.9 to 10.0 1/eV*f.u. for $BaPt_3AuGe_{12}$ and thus should also increase T_c (experimental and theoretical full-relativistic results for Ba are in ref. [5]).

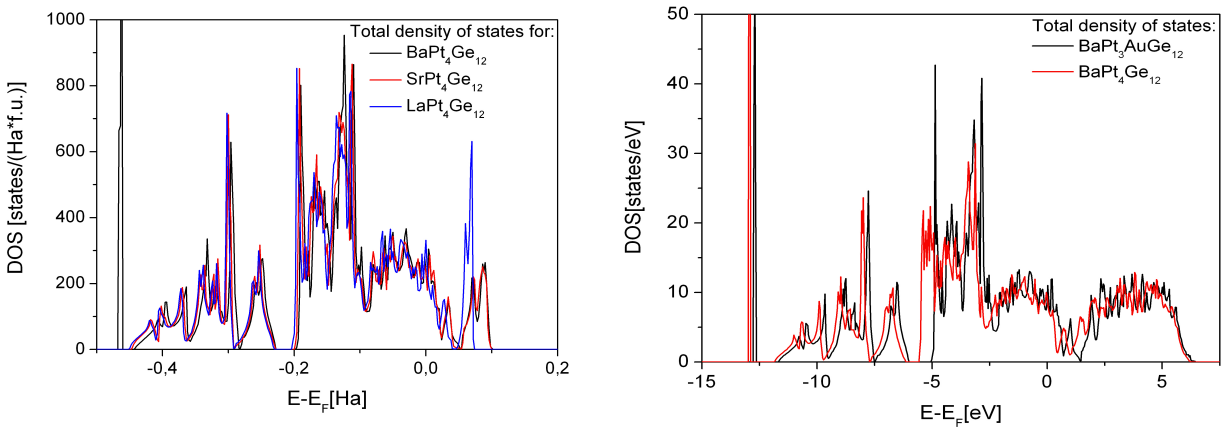

Fig.1. Left: Total density of states (DoS) for MPt_4Ge_{12}, M=Ba, Sr, La, obtained from full-potential LAPW method (elk) for experimental crystalographic data. Right: Total DoS for $BaPt_4Ge_{12}$ with and without gold substitution for theoretical lattice constants within PAW method (VASP).

References

1. E. Bauer *et al.*, Phys. Rev. Lett. **99**, 217001 (2007)
2. R. Gumeniuk *et al.*, Phys. Rev. Lett. **100**, 017002 (2008)
3. D. Kaczorowski *et al.*, Phys. Rev. B **77**, 180504 (R) (2008)
4. E. Bauer *et al.*, Phys. Rev. B **78**, 064516 (2008)
5. R. Gumeniuk *et al.*, Phys. Rev. B **78**, 052504 (2008)
6. D. H. Galvan, Journal of Superconductivity and Novel Magnetism **22**, 367 (2009)
7. V. H. Tran *et al.*, Phys. Rev. B **79**, 054520 (2009)
8. V. H. Tran *et al.*, Phys. Rev. B **79**, 144510 (2009)
9. H. Rosner *et al.*, Phys. Rev. B **80**, 075114 (2009)