ELECTRONIC DENSITY OF STATES OF YTTRIUM IRON GARNET

Ryszard J. Wojciechowski[a],**A. Lehmann-Szweykowska**[a], **Roman Micnas**[a], **and Gillian A. Gehring**[b]

[a]A. Mickiewicz University, Institute of Physics, ul. Umultowska 85, 61-614 Poznań, Poland

[b]Department of Physics and Astronomy, University of Sheffield, Sheffield S3 7RH, UK

9.7 cm

We have calculated the electronic structure of $Fe^{3+}O_4^{2-}$ (tetrahedral) and $Fe^{3+}O_6^{2-}$ (octahedral) clusters. Molecular-orbital point-symmetry cluster calculations have proven useful for providing insight into the real-space crystal unit cell consisting of 20 iron-oxygen clusters. Discrete energy levels calculated with the point symmetry group S_4 and S_6, respectively, are broadened due to charge-particle symmetry permitted inter-cluster motion. The transfer probability of spin up or down hole is energetically inequivalent. The on-site Coulomb repulsion on the iron ions is responsible for the spin dependance of the charge transport. The electronic DOS turns out to consist of narrow-bands.

[1] C. Srintiwarawong and G.A. Gehring, J. Phys.: Condens. Matter **13**, 7987 (2001).

[2] A. Lehmann-Szweykowska, T. Lulek and M.M. Kaczmarek, J. Phys.: Condens. Matter **13**, 3607 (2001).

13.4 cm

Subject category :

3. Transition Metals, Alloys and Compounds

Presentation mode :
oral

Corresponding author :
Ryszard J. Wojciechowski

Address for correspondence :
A. Mickiewicz University, Institute of Physics
ul. Umultowska 85, 61-614 Poznań, Poland

Email address :
wojrysz@main.amu.edu.pl