

Comment

Comment on Phys. Rev. B paper: "Surface effects in the Ni 2p x-ray photoemission spectra of NiO" - the strength of the crystal field in NiO.

R. J. Radwanski*

*Center of Solid State Physics; S^{nt} Filip 5, 31-150 Krakow, Poland
Institute of Physics, Pedagogical University, 30-084 Krakow, Poland*

(reprint ActAPhysica **23-24** (2008) 28,
under the law protection of Phys. Rev. B from 6 June, 2008, BTK1007;
related to Acta Phys. Pol. A **97**, 963 (2000);
First-principles description of NiO - see Acta Physica 1 (2006) 26;
published 31 July 2009; online: www.actaphysica.eu)

By this Comment we would like to express our deep scepticism about the strength of the crystal-field parameter in NiO taken in Ref. [1] into calculations, $10Dq$ of 0.1 eV. This value is written twice, in Table 1 and on page 3, right column top. We claim that this value is more than 10 times too small. We claim that the correct value of $10Dq$ in NiO is 1.08 eV.

A value of $10Dq$, an promotion $t_{2g}-e_g$ energy, is fundamental parameter for any description of properties of NiO. There is a wide literature on this subject. Quite extensive reference list can be found in our papers, see for instance [2, 3].

Moreover, the authors considering "the ground state expanded in the $3d^8$, $3d^9L$ and $3d^{10}L^2$ configurations" do not give the obtained contributions what is essential for any scientific discussion of the results.

In conclusion, we claim that a value of 0.1 eV taken in Ref. [1] for the strength of the octahedral crystal-field $10Dq$ in NiO is in a sharp disagreement with well-established experimental value of 1.1 eV. Moreover, it is a pity that the authors do not specify the ground state of the Ni ion in NiO taken into calculations.

-
- [1] L. Soriano, I. Preda, A. Gutierrez, S. Palacin, M. Abbate, and A. Vollmer, Phys. Rev. B **75**, 233417 (2007).
[2] R. J. Radwanski and Z. Ropka, Acta Physica **1**, 26 (2006); www.actaphysica.eu.
[3] R. J. Radwanski and Z. Ropka, arXiv:cond-mat/0606604 (2006).

* <http://www.e-physica.pl>; Email: sfradwan@cyf-kr.edu.pl