

**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.**

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First-principles description of NiO - see Acta Physica 1 (2006) 26;  
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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.

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- [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](http://www.actaphysica.eu).  
[3] R. J. Radwanski and Z. Ropka, arXiv:cond-mat/0606604 (2006).

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