Comment

Comment on Phys. Rev. Lett. paper: "Metal-Ligand interplay in strongly correlated oxides: A parametrized phase diagram for pressure-induced spin transitions" - the strength of the crystal field in NiO.

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By this Comment we would like to express our deep scepticism about the strenght of the crystal-field parameter in NiO taken in Ref. [1] into calculations, $10Dq$ of 0.3 eV (Table 1). We claim that this value is more than 3.5 times too small. We claim that the correct value of $10Dq$ in NiO is 1.09 eV. We would suppose that the value of $10Dq$ does not influence the high energy spectra.

Despite of writing this Comment we fully appreciate research by Mattila *et al.* [1] as a step towards the scientific truth. We are forced to write a Comment by an unscientific policy of Editors of Phys. Rev. Lett. finding *a priori* my papers on NiO, describing the magnetism and low-energy electronic structure within a very-strongly electron-correlated limit with substantial importance of the detailed crystal field and spin-orbit coupling, as unsuitable for publication in Phys. Rev. Lett. by last ten years.

A value of $10Dq$, an promotion t_{2g}-e_g energy, is fundamental parameter for any description of properties of NiO. Van Elp and Tanaka [2] have written already 10 years ago that "Probably the most important parameter is the ionic $10Dq$ splitting." (p. 5333). I fully agree with this statement. There is a wide literature on this subject. Quite extensive reference list can be found in our papers, see for instance [3, 4]. For a scientific honesty I have to mention that in a quite recent paper Soriano *et al.* [5] have assumed only 0.1 eV for $10Dq$, whereas Taguchi *et al.*

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[6] a value of 0.3 eV. We have been submitted our Comments to both these papers [7, 8].

Moreover, for the authors of Ref. [1] "the ground state is described by linear combination of $3d^8$, $3d^9\mathrm{L}$, $3d^{10}\mathrm{L}^2$ ... configurations", page 2, right column. The authors do not give, however, the used/obtained contributions. It unables any scientific discussion of the results.

In conclusion, we claim that a value of 0.3 eV taken in Ref. [1] for the strength of the octahedral crystal-field $10Dq$ in NiO is in a sharp disagreement with a well-established experimental value of 1.09 eV. Moreover, it is a pity that the authors do not specify the ground state of the Ni ion in NiO taken into calculations. It is a future task to combine such theoretical approaches as that presented in Ref. [1] for high-energy excitations with the many-electron crystal-field theory (QUASST), which adequately describes zero- and low-temperature properties including formation of the magnetic state, low-energy electronic structure (< 1.5 eV) and termodynamics.

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