Comment on "Atomic Many-Body Effects for the p-Shell Photoelectron Spectra of Transition Metals"

Recently, Bagus *et al.* [1] reported an *ab initio* relativistic many-body calculation of $2p$ and $3p$ x-ray photoemission spectra (XPS) for a Mn^{2+} ion, and concluded that their atomic model was able to explain most of the features in the XPS of MnO. In discussing the result, they referred to our previous cluster model (CM) calculations [2,3] with the charge transfer (CT) effect, but they made serious misconceptions on our calculations.

In order to make the point clear, we have calculated the Mn $2p$ and $3p$ XPS with our CM but by disregarding crystal field (CF) and CT effects. The results are shown with solid curves in Figs. 1(a) and 1(a′) and compared with those by Bagus *et al.* (solid circles). In our calculation, we used the standard atomic multiplet theory [4] and no empirical adjustments were made to the term-averaged Hartree-Fock values of Slater integrals for the $3d^5$, $2p^5 3d^5$, and $3p^5 3d^5$ configurations. We used the same Lorentzian and Gaussian broadenings as those of Ref. [1]. It is clear that two calculations give almost the same results. Bagus *et al.* stressed the importance of the d shell angular momentum (AM) recoupling effect, and stated in the abstract of Ref. [1] that a combined treatment of relativity and electron correlation reveals important physical effects that have been neglected in virtually all previous work. However, essentially the same effects were already taken into account in our previous publications [2,3] by a different method. We note that our result in Fig. 1(a) is almost the same as that in Fig. 3 of the previous paper [2] except for the reduction of Slater integrals.

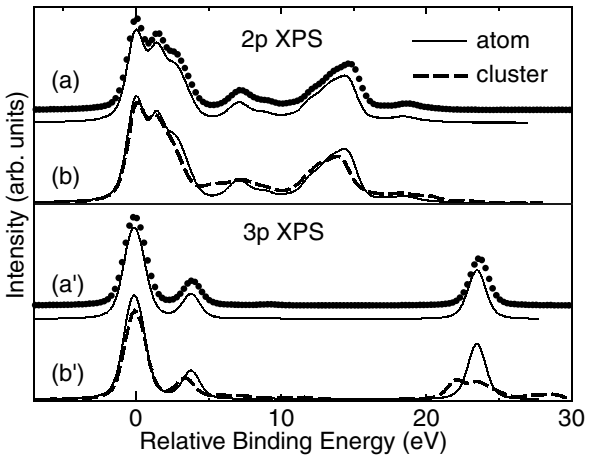

FIG. 1. Calculations of the Mn $2p$ (top part) and $3p$ (bottom part) XPS of MnO using an atomic model (solid lines) and atomic + CF + CT model (dashed lines). The parameters are given in Ref. [3]. The solid circles are taken from Ref. [1].

The main purpose of our previous papers [2,3] is to study the interplay between CT and atomic multiplet effects for various transition metal compounds. The CT effect is small in MnO compared with other compounds, but still important (see Refs. [2,3]). We show in Figs. 1(b) and 1(b′) (dashed curves) the results of our CM calculations with CF (CF effect is very minor in this case). When the CT effect is switched on, the spectral shape of the satellite at about 6 eV of $2p$ XPS is strongly modified, and for the $3p$ XPS the exchange satellites at the high-binding energy side are drastically changed. By this CT effect the agreement with the experimental results is improved (compare them with the experimental data in Ref. [1]). Bagus *et al.* misunderstood from our previous CM [3] that the second and fourth satellites of $2p$ XPS and the first satellite of $3p$ XPS were caused by the CT mechanism. It is evident from Fig. 1 that they arise mainly from atomic multiplet structures. We stress that the d shell AM recoupling effect was already taken into account in our calculations [2,3].

Finally, we mention that the effects of a reduction of Slater integrals and a term-dependent core hole lifetime are important to obtain a better agreement with the experimental results. These effects were included in our previous CM [2,3], but not taken into account in the *ab initio* calculation by Bagus *et al.*

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