

# Additions and Corrections

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**D. Dai, M.-H. Whangbo, J. Köhler, C. Hoch, and A. Ville-suzanne:** Electronic Structure Analysis of the Difference between  $\text{Cs}_2\text{AgF}_4$  and  $\text{Rb}_2\text{MnF}_4$  in Their Magnetic Properties and Single-Crystal Structure Determination of  $\text{Rb}_2\text{MnF}_4$ .

Please note the following correction to this article (*Chem. Mater.* **2006**, *18*, 3281).

This paper (*Chem. Mater.* **2006**, *18*, 3281) examined why the two magnetic insulators  $\text{Cs}_2\text{AgF}_4$  and  $\text{Rb}_2\text{MnF}_4$  differ in their magnetic properties, namely, why the intralayer spin exchange is ferromagnetic in  $\text{Cs}_2\text{AgF}_4$  but antiferromagnetic in  $\text{Rb}_2\text{MnF}_4$ . In this study, the ferromagnetism in  $\text{Cs}_2\text{AgF}_4$  was found to arise from the spin polarization of the  $d_{x^2-y^2}$  bands, which is induced by the  $d_z^2-p-d_{x^2-y^2}$  orbital interactions of the Ag–F–Ag bridges in the  $\text{AgF}_2$  layers of  $\text{Cs}_2\text{AgF}_4$ . The presence of such interactions implies that substantial covalent bonding exists in the Ag–F bonds. In this context, the work missed citing the papers by Grochala and Hoffmann<sup>1</sup> and by Grochala et al.,<sup>2</sup> which discussed the existence of covalent bonding in the Ag–F bonds of numerous silver fluoride compounds, including  $\text{Cs}_2\text{AgF}_4$ . They described the electronic structure of  $\text{Cs}_2\text{AgF}_4$  on the basis of non-spin-polarized DFT calculations, hence predicting that  $\text{Cs}_2\text{AgF}_4$  is a metal. We thank Professor R. Hoffmann for informing us of the relevance of these two papers to our work.

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(1) Grochala, W.; Hoffmann, R. *Angew. Chem., Int. Ed.* **2001**, *40*, 2742.

(2) Grochala, W.; Egdell, R. G.; Edwards, P. P.; Mazej, Z.; Zemva, B. *ChemPhysChem.* **2003**, *4*, 997.

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