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Susan Biering,[†] Andreas Hermann,[†] Jürgen Furthmüller,[‡] and P. Schwerdtfeger*[,†]: Erratum: The Unusual Solid-State Structure of Mercury Oxide: Relativistic Density Functional Calculations for the Group 12 Oxides ZnO, CdO and HgO

Page 12427.

The spin−orbit coupled results were obtained as a nonvariational correction to the scalar relativistic one-particle density. A program error resulted in incorrect band structures for the spin−orbit coupled case. The bottom pictures of Figures 4 and 5 in the original publication[1] are therefore incorrect, and the variational spin−orbit corrected results for the band structure and density of states are now given in Figures 1 and 2 below. The discussion changes insofar as the inclusion of spin−orbit coupling does not alter the electronic properties to a metallic behavior originally blamed on the density functional. Instead, the band gap is maintained but slightly decreased to 1.17 eV.

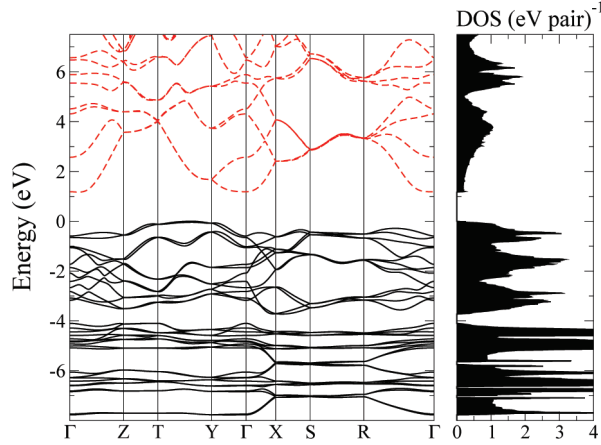

Figure 1. Band structure and density of states for HgO, relativistic montroydite structure including spin−orbit coupling. The valence band maximum and the Fermi energy respectively is set to zero energy. The black solid lines indicate the valence, and the red dashed lines are the conducting bands.

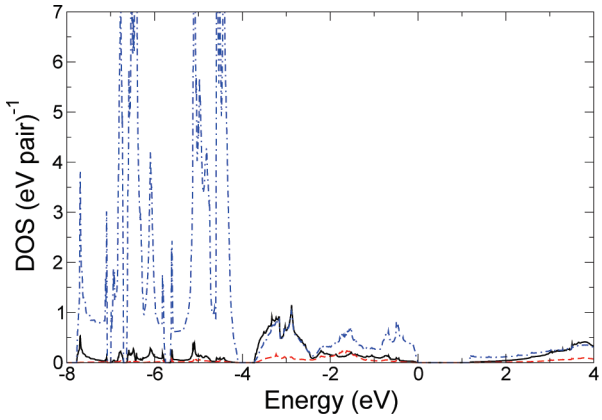

Figure 2. Site-projected density of states for HgO relativistic montroydite including spin−orbit coupling. The black solid, red dashed, and blue dash-dotted lines indicate the s, p, and d site-projected DOS respectively.

References and Notes

(1) Biering, S.; Hermann, A.; Furthmüller, J.; Schwerdtfeger, P. *J. Phys. Chem. A* **2009**, *113*, 12427.

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