# Chemical Bonding in Metallic Rutile-type Oxides $TO_2$ ($T$ = Ru, Rh, Pd, Pt)

Gérard Demazeau[a], Samir F. Matar[a], and Rainer Pöttgen[b]

[a] ICMCB – CNRS, Université Bordeaux 1, 87, Avenue du Docteur A. Schweitzer, 33608 Pessac Cedex, France
[b] Institut für Anorganische und Analytische Chemie, Universität Münster, Corrensstraße 30, D-48149 Münster, Germany

Reprint requests to S. F. Matar. E-mail: matar@icmcb-bordeaux.cnrs.fr

*Z. Naturforsch.* **2007**, *62b,* 949 – 954; received April 4, 2007

*Dedicated to Dr. Bernard Chevalier on the occasion of his 60$^{th}$ birthday*

Synthesis routes to rutile-type oxides with 4*d* and 5*d* transition elements are summarized. Trends in electronic structure have been established through an analysis in the framework of density functional theory presenting the band structure, the density of states and the properties of chemical bonding. The metal-oxygen bond is found to play the major role in bonding of the system in the valence band. Throughout the series $4d \rightarrow 5d$ ($RuO_2$, $RhO_2$, $PdO_2$ and $PtO_2$) the crystal field analysis of the band structure shows a lowering of $e_g$ towards $t_{2g}$ manifolds and a broadening of the overall density of states. In the vicinity of the Fermi level the role of the antibonding metal-oxygen character is investigated in the context of instability towards possible magnetic polarization, especially for $RuO_2$.

*Key words:* Oxides, $RuO_2$, $RhO_2$, $PdO_2$, $PtO_2$, Rutile-type, DFT