

Structural and Electronic Trends in Rutile Compounds

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Rutile structure is ubiquitous in transition metal (TM) dioxides: All but two early TM dioxides at least have an polymorph that has either the rutile structure or a slightly distorted variant of it. Ideal, tetragonal rutile structure involves TM ions at the center of almost perfect oxygen octahedra, which form edge sharing chains. A common, slightly distorted variant of the rutile structure is the so called MoO₂ structure, which involves cations forming pairs along these edge sharing octahedron chains. While there are various studies on individual compounds and why they form in undistorted rutile or the MoO₂ structures, there is no single study that explains the structural trends in early TM dioxides.

In this work we present a complete study of structural and electronic trends in early TM dioxides. We show how the interplay of a pseudo-Peierls mechanism, proposed as the driving force for the dimerization in compounds like VO₂ [1] or MoO₂ [2], with structural degrees of freedom lead to rich, nonmonotonic trends in these compounds. This provides a beautiful example of how electronic structure can lead to structural changes in the well known rutile structure.

This work is supported as part of the Energy Materials Center at Cornell (EMC²), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Grant No. DE-SC0001086.

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