

UW and IFJ theoreticians explain crystal structures of transition metal monoxides

Transition metal monoxides *i.e.* chemical compounds of the formula MO are often found in nature and they have been used as early as in Neolithic period for pottery - and later glassware - colouring. These important materials exhibit a great variety of physical properties such as diverse electronic and thermal conductivity, magnetic or optical features, and they find numerous daily life applications. Nearly twenty MOs have been prepared to this day and even more wait to be synthesized. It has long been known that most of them crystallize in the prototypic rock salt (NaCl) structure – either undistorted or only slightly distorted due to magnetic interactions operating at low temperatures. This important cubic structure is frequently found for inorganic compounds, especially ionic ones. But five oxides: those of copper, silver, palladium, platinum and mercury, do not fit the family since they adopt much more complex lower-symmetry structures. Still, do they have anything in common with the cubic ones?

In their letter Dr Mariana Derzsi and Prof. Wojciech Grochala from the University of Warsaw joined by their colleague, Prof. Przemyslaw Piekarczyk from the Institute of Nuclear Physics in Cracow (Poland) described the state-of-the-art theoretical calculations carried out for the five oxides in question. These quantum mechanical studies employed very precise but computer power-demanding hybrid density functional theory calculations. Each of five MOs computed has proved to be unstable in the rock salt structure since *for all of them an imaginary phonon mode appears at the same point of the first Brillouin zone, $L=(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$* . And this instability turns out to lead to the factual crystal structures they adopt at low temperatures.

Thus, the researchers have managed to explain the origin of the complex crystal structures taken by copper, silver, palladium, platinum and mercury oxides as coming from the much simpler cubic precursor. This has permitted them to rationalize the similarities in the crystal structures of all transition metal oxides which had been noticed previously (M. Derzsi *et al.*, *Eur. J. Inorg. Chem.* (29): 5095-5102 2013). Interestingly, diverse mechanisms of electron-phonon coupling turned out to yield the observed structural diversity.

According to the authors, the "phonon instability" mechanism should be viewed as a very general one. It could now be used to rationalize a great number of complex crystal structures known experimentally for the chemical elements and compounds.

The article “*Structures of late transition metal monoxides from Jahn-Teller instabilities in the rock salt lattice*” will be published in *Physical Review Letters*. The calculations were carried out at the Interdisciplinary Center for Mathematical and Computational Modeling of the University of Warsaw (ICM) with the extensive use of Medea package and took over one year.

