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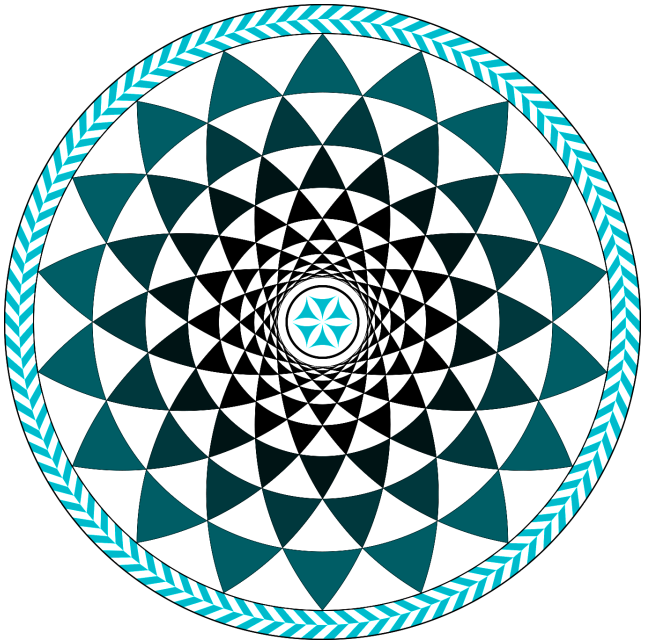

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Local structure studies of multifunctional $CuMoO_4$ and $CuWO_4$ solid solutions

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Copper molybdate ($CuMoO_4$) and related solid solutions are multifunctional materials exhibiting several chromic-related properties, including thermochromism, tribochromism, piezochromism, halochromism. $CuMoO_4$ also has thermosalient, photoelectrochemical, catalytic and antibacterial features. To control the functionality of the material, its structure-property relationship must be understood.

In this study, $CuMo_{1-x}W_xO_4$ thermochromic compounds were investigated to elucidate the structural origin of their optical properties. The results of temperature and composition-dependent X-ray absorption and resonant X-ray emission spectroscopy (XAS and RXES) studies are presented. XAS provides information on the local environment around absorbing atoms. Reverse Monte-Carlo calculations allowed us to create a 3D structural model consistent with the experimental data and to follow a change of the local structure of $CuMoO_4$ upon temperature variation. The RXES method was used to understand the role of W^{6+} ions in $CuMo_{1-x}W_xO_4$ solid solutions and determine changes in the crystal field-induced splitting of the 5d(W) states across the phase transitions.

The ability to adjust the thermochromic properties in a controllable manner to more desired temperature ranges may make the material interesting for applications as an indicator for monitoring storage/processing conditions of temperature-sensitive products (drugs, vaccines, chemicals, biological materials, etc.).

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