Y-H-O CHROMOGENIC SYSTEMS: DESIGN, CRYSTAL CHEMISTRY ASPECTS, AND STRUCTURE-PROPERTY RELATIONSHIPS

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Yttrium oxyhydride (Y-H-O) systems represent an interesting class of novel functional materials exhibiting unusual chemical, physical and optical properties. We present our theoretical results on atomic-scale crystal assembly and modeling of these compounds. The fundamental aspect of our work is that we described the crystal chemistry of the Y-H-O systems from the point of view of variable oxygen content. In this context, the structure-chemical-composition dependences were expressed via step-wise oxidation process governing the formation of different crystalline phases. In the scenario of the partial oxidation process, we indicated the effect of spatial separation of the Y-O and Y-H chemical interactions, and the effect of long-range oxygen orderings. On the base of stable lattice geometries we carried out the simulations of structural, elastic, vibrational, electronic, and optical properties. Successful comparison with experimental data and observations has been made. In particular, we analysed the possibility of manipulation of oxygen content in the chemical composition to control mechanical, electronic and chromogenic properties.

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