

DESIGN OF NOVEL MATERIALS ON THE BASE OF RARE-EARTH METAL OXYHYDRIDES

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Mixed-anion systems in which rare-earth metal atom is coordinated both by oxygen and one or more anion species present a new promising class of materials that can exhibit a number of useful properties. In the context of creating materials with interesting properties we performed theoretical studies of the rare-earth metal oxyhydrides. We present the current progress, status and directions for the future research of this group of mixed-anion materials which can be suitable for applications in solid-state and power electronics. We have shown that the charge-ordering and cooperative charge-localization effects in the oxyhydride compounds underly the formation of stable structures with remarkable piezoelectric and ferroelectric properties. From our theoretical analysis follows that the given systems can be used as functional components in the design of high sensitivity piezoelectric sensors and actuators, high performance ferroelectric random-access memory and nanosized ferroelectric tunnel junctions.



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