Poster

$BaCoO_2$ with Tetrahedral Cobalt Coordination: Unlocking Energy Storage and Conversion in $BaCoO_3$-δ Materials

Jerome Rouquette

(ICGM Universite de Montpellier)

jerome.rouquette@umontpellier.fr

Barium-cobaltate-based perovskites ($BaCoO_3$-δ) and barium-cobaltate-based nanocomposites have been extensively studied for energy storage and conversion devices due to their flexible oxygen stoichiometry and tunable oxidation states of non-precious transition metals. Despite a wide array of structural polymorphs reported for these perovskites, the potential structural changes during the oxygen reduction and oxygen evolution reactions have not been investigated. In this study, we synthesized and characterized $BaCoO_2$, the compound's lowest possible Co-oxidation state, which exhibits a quartz-derived trigonal structure with a helicoidal corner-sharing CoO_4-tetrahedral framework, as proposed by Spitsbergen et al. Oxygen can be reversibly inserted into this crystal structure to form $BaCoO_3$-δ ($0 \leq \delta \leq 1$), based on results from an in-situ coupled thermogravimetric-neutron diffraction study. This reveals a giant oxygen storage capacity due to the extreme tunability of the cobalt cations' electronic configuration, which is fundamental to the material's performance. The reversible conversion of $BaCoO_2$ to $BaCoO_3$-δ, along with similar electronic conductivity above 900 K, highlights the high potential of $BaCoO_3$-δ-based devices for energy storage and conversion.