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BOOK OF ABSTRACTS

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Band gap engineering in novel fluorite-type rare earth high-entropy oxides (RE-HEOs) with computational and experimental validation for photocatalytic water splitting applications

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Five different rare-earth-based nanocrystalline high entropy oxides (HEOs) with fluorite type of structure and average crystallite sizes between 6 and 8 nm were prepared and their photocatalytic behaviour towards AZO dye degradation and photoelectrochemical water splitting for hydrogen generation was examined. The cationic site in the fluorite lattice consists of five equimolar elements selected from the group of rare-earth elements including La, Ce, Pr, Eu, and Gd and second-row transition metals, Y and Zr. Studied HEOs exhibit bandgaps in the range from 1.91 eV to 3.0 eV and appropriate valence and conduction bands for water splitting. They reveal high photocatalytic activity that is mostly attributed to the accessibility of more photocatalytic active sites which provided radicals responsible for the AZO dye degradation. The materials successfully produce hydrogen by photocatalytic water splitting, suggesting the potential of HEOs as new photocatalysts. The photocatalytic performances of all studied HEOs outperform the single fluorite oxides or equivalent mixed oxides. The $Ce_{0.2}Zr_{0.2}La_{0.2}Pr_{0.2}Y_{0.2}O_2$ (CZLPY) engender hydrogen in 9.2 μmolmg^{-1} per hour that is much higher content than for pristine CeO_2 material which amounts to 0.8 μmolmg^{-1} per hour. The explanation of the obtained experimental results is supported by density functional theory (DFT) calculations. The density of states (DOS) and the projected DOS after high-entropy equimolar doping (CZLPY) of starting pristine CeO_2 indicated that the bandgap is significantly reduced from 3.48 to 2.71 eV due to Pr 4f and O 2p orbital mixing. DFT calculation also disclose that a strong interaction between AZO dye methylene blue (MB) and CZLPY(111) is responsible for observed higher photodegradation of MB by CZLPY compared to pristine CeO_2. This occurs due to the existence of three solid bondings of MB with the surface of CZLPY(111) compared to only one solid bonding with the surface of CeO_2 (111).

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