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FP-LAPW based first principles study of RAlO3 (R = Dy and Tb) using density functional theory: A GGA+Ustudy

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Density functional theory (DFT) based calculations of electronic and magnetic properties of RAlO3 (Dy and Tb) have been performed using FP-LAPW method within the framework of the LSDA+U approach. There are-earth aluminates have attracted much attention because of the presence of the highly localized f-electrons of rare-earth, with high density of states near Fermi level. The calculations performed near the Fermi level of density of states shows the compound to be suitable for thermoelectric application. The exchange-splitting of R-4f states were analysed to explain the behaviour of RAlO3.

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Fully printable mesoscopic solar cells: From dye-sensitized to perovskite

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Since the first report in 1991, Dye-Sensitized Solar Cells (DSSCs) have been recognized as a promising alternative to commercial silicon solar cells due to their low fabrication cost and relatively high conversion efficiency. A typical DSSC contains a sensitized-TiO2 photoanode, a liquid electrolyte and a platinum plate counter electrode. However, DSSC based on liquid electrolyte have many practical problems such as leakage, desorption of dye, erosion of electrode, which blocks its rapid commercial application. Replacing the liquid electrolyte with a solid-state medium seems to be a solution to these problems. Up to now, the highest efficiency up to 17.9% has been attained with the solid-state-DSSCs assembling with lead iodide perovskite inorganic sensitizers and 7.2% with a new organic D-π-A dye. Unfortunately, the counter electrode of the conventional all-solid-state DSSC is made by evaporating Au or other noble metals, which needs not only expensive noble metals but also costly equipment for high vacuum. Obviously, a low cost counter material and simple technology expects to be developed urgently. With the mesoscopic carbon counter electrode, we developed a stable mesoscopic perovskite solar cells with simpler manufacturing process based on full screen-printing technology with an efficiency of 15.6%, which offers a promising prospect for its commercial application.

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