

Chemical Mapping of High-Temperature Deposited NiOx with XPS

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Non-stoichiometric nickel oxide (NiOx) is a promising inorganic hole transport layer (HTL) for perovskite solar cells (PSCs). Here, we investigate the evolution of chemical species and optoelectronic properties in ultra-thin NiOx films deposited via ion beam sputtering (IBSD) under varied thermal and oxidative treatments. We demonstrate that p-type conductivity, transparency, and band alignment in NiOx are governed directly by the concentration of Ni³⁺ related to nickel vacancies. Additionally, UV/Ozone exposure is shown to introduce NiOOH, enhancing surface wettability and increasing the work function by the creation of a surface dipole, improving charge extraction but reducing long-term stability of NiOx films due to hygroscopic decomposition. High temperature deposition at 300 °C yields the best balance between opto-electronic properties, recombination and most stable surface chemistry, yielding the best photo voltaic performance among tested conditions.