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PhD THESIS DEFENSE: Environmentally-friendly perovskite nanocrystals based on titanium and tin

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The availability of energy is a fundamental ingredient for the development of society. However, the intense consumption of fossil fuels as an energy resource since the second industrial revolution has caused a massive increase in the concentration of CO2 and other greenhouse gases in the atmosphere, which is nowadays known to be the first cause of climate catastrophe. For this reason, it has become a priority to replace fossil fuels with more sustainable sources, which are renewable and produce low greenhouse gas emissions. Photovoltaics is one of the suitable technologies to carry out this fast transition because it is already well-developed and is based on the use of the infinite energy source, the Sun. However, increasing the efficiency of solar light conversion into electricity and reducing the cost of photovoltaic devices is fundamental to achieve the goals set by policy makers.

Consequently, the development of novel optoelectronic materials, based on abundant and environmentally friendly elements, is one of the fundamental scientific advances needed to boost the shift towards a low-carbon society.
Perovskites, whose solar cells reached this year a certified record efficiency of 25.7%, are the first solution-processed materials to outperform multicrystalline and thin-film silicon and therefore one of the most interesting new materials for photovoltaic applications. In spite of their astonishing performances in solar cells, the most promising perovskites contain lead, which is toxic for human beings and potentially a threat to the environment. Hence, over the last decade, there has been intensive research on strategies to replace lead in the perovskite structure with nontoxic elements. Among all the novel perovskites studied, titanium-based vacancy-ordered double perovskites demonstrated one of the most promising performances when applied in solar cells.
This thesis focuses on the development of new solution syntheses for the preparation of novel lead-free vacancy-ordered double perovskite nanocrystals based on titanium and tin in the oxidation state +4, which are nontoxic and abundant elements. All the synthesized perovskite nanocrystals were characterized structurally, chemically and optically. Moreover, the experimentally observed optical properties and the stabilities of these materials were further confirmed by ab initio density functional theory calculations.
We initially developed a colloidal synthesis to prepare mixed bromide-iodide Cs2TiBr6?xIx perovskites. All these materials are intrinsically stable with bandgaps in the visible region; suitable for solar cell applications. However, they showed very high instability in air, which prevented their application in devices and that motivated us to search for strategies to stabilize them.
Encouraged by the higher reported stabilities of Sn+4 perovskites with the same vacancy-ordered double perovskite structure, we synthesized pure tin halide perovskite NCs and novel mixed titanium/tin iodide and bromide perovskite NCs. The experiments confirmed that tin perovskites are stable in air and that the mixtures with the highest amount of tin in the structure are stable in air for longer than pure titanium perovskites. Finally, for the case of Cs2TiBr6, we developed a room temperature method to reach comparable stabilities in air through a surface treatment with tin compounds.
In summary, we have developed a low-temperature solution method for the preparation of novel environmentally-friendly perovskites based on tin and titanium and studied their properties for the first time, both computationally and experimentally. Finally, we have found a way to increase the stability in air of titanium-based perovskites through the addition of tin in the structure. Overall, this thesis provides an insight into novel lead-free perovskites based on titanium and tin and it represents a milestone for the understanding and development of this new class of materials.
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