

Electronic and excitonic properties of MAPbSnI₃ perovskite alloys

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MAPb_xSn_{1-x}I₃ alloys are promising for photovoltaic, optoelectronic, and spintronic applications [1,2,3]. At the heart of perovskite solar cell technologie lies methylammonium lead iodide (MAPI), a key organic–inorganic perovskite that adopts a tetragonal structure at room temperature with a direct bandgap of 1.6 eV. Substituting lead with tin in MAPI addresses environmental concerns and decreases energy bandgap but introduces challenges, including lower power conversion efficiencies, and reduced chemical stability due to the oxidation of Sn²⁺. A potential solution is the partial substitution of lead with tin, yielding alloys like MAPb_xSn_{1-x}I₃. Beyond photovoltaics, lead halide perovskites also show great promise in spintronics. These materials exhibit spin-selective optical transitions and tunable spin–orbit coupling (SOC), which can be adjusted by varying the halogen or metal components. Specifically, substituting lead with tin reduces SOC strength, leading to longer spin relaxation times, a key parameter for spin- tronic devices.

We determined their fundamental band parameters of these alloys as a function of Pb content (x) by using $k \cdot p$ calculations []. The main excitonic properties are also calculated. In agreement with experimental results [5], we consider the P4mm structure for Sn-rich alloys and I4cm for Pb-rich alloys.

Our model reproduces the non-monotonic band gap behavior and provides detailed insights into the electron, hole, and exciton masses. Hole masses are slightly larger than electron masses, both increasing linearly with x , with a discontinuity at $x = 0.5$ due to the structural transition. The calculated exciton masses align well with experimental data [6].

We also predict the Landé g -factors for charge carriers and excitons. In Pb-rich alloys, g_e increases as the band gap decreases, whereas in Sn-rich alloys, it decreases. Exciton g -factors (g_x) vary with composition, ranging from 2.4 to 4.8 for Pb-rich alloys and 4.8 to 3.7 for Sn-rich alloys.

These findings highlight the tunable electronic and spin properties of MAPb_xSn_{1-x}I₃, making them strong candidates for next-generation devices.

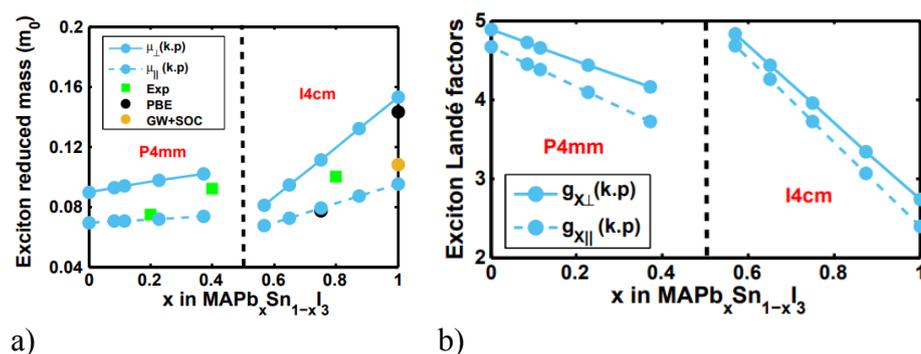


Figure 1 Excitonic properties versus lead content in MAPbSnI₃ alloys. \parallel and \perp means along and perpendicular to the tetragonal axis of the crystal a) Dependence of the reduced exciton masses Exp ref[5] and PBE or GW+SOC calculations ref. [7] and [8] respectively.

b) Dependence of exciton Landé factors

References

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