An experimentally-validated multi-scale materials, process and device modelling & design platform enabling non-expert access to open innovation in the Organic and Large Area Electronics Industry (MUSICODE)

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PU	Public	
PP	Restricted to other programme participants (including the Commission Service)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (excluding the Commission Services)	x

Deliverable author(s): Cameron Underwood, Dimitar Kutsarov and Ravi Silva (USUR)

Contributors

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Consisting of Coordinator:	University of Ioannina (UoI)	Greece
Partners:	Karlsruhe Institute of Technology (KIT)	Germany
	University of Surrey (SURREY)	UK
	Aristotle University of Thessaloniki (AUTh)	Greece
	Czech Technical University in Prague (CVUT)	Czechia
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	Apeva SE (APEVA)	Germany
	AIXTRON SE (AIXTRON)	Germany

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Publishable summary

There is no doubt that Perovskite-based Photovoltaics (PV) will enter the PV marketplace very soon. This originates from their unique properties, such as band gap tunability and high absorbance coefficient, making them suitable for indoor applications, vacuum- and/or solution processability, high power conversion efficiency (PCEs), and many more. While a non-certified PCE of only 2.8% was reported in 2009 for perovskite solar cells (PSCs), the current certified PCE record for a single junction PSCs is 25.8%. Notably, this PCE is higher than the highest reported for a single junction multi-crystalline PV (24.4%), which is the most wide-spread silicon-based PV technology nowadays. Recently (stand April 2023), KAUST reported a certified PCEs of 33.2% for a tandem perovskite/Si device, which again is higher than recently reported PCE for a Si-based multijunction device (32.9%). Clearly, PSCs show an unprecedented PV technology development step in terms of PCE. Giant improvement leaps have also been achieved in terms of the operation stability of the PSCs and reports of a successful passing of IEC testing standards such as ISOS-L2 and ISOS-D3 have been shown.

Although various material systems have been studied, theoretically there are many possible two-dimensional perovskite systems of the form $PEA_2Ge_{1-x}Sn_xI_4$, where x = 0, 0.25, 0.5, 0.75 and 1 which have not been explored yet. Hence, in this report we use plane-wave DFT calculations to gather insight into theoretical properties of such perovskite systems. We show that these systems show a nonlinear trend of band gap as a function of Sn content, where $PEA_2Ge_{1-x}Sn_xI_4$ shows a minimum at a predicted x = 0.725 and a band gap of 1.945 eV. The behaviour of the electronic structure is consistent between the Pb-Sn and Ge-Sn systems, although there is a difference in the band gap bowing; this is attributed to the smaller ionic radius of Ge as compared to Pb and is thus a measure that can be used to control the nonlinear trend of band gap as a function of Sn content. Overall, this work contributes to the understanding of the electronic properties of perovskite systems and gives insights into the possibility of fabricating Ge-Sn based Ruddlesden-Popper perovskites in future electronic devices.