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## **Materials design of halide perovskites and beyond: Opto-electronic properties, and charge carrier mobilities from first principles.**

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Ab initio calculations are becoming more and more efficient and have emerged as an indispensable tool to model, characterise and understand complex systems like halide perovskites and perovskite-like materials. In particular, over the last decade, such computational approaches have been extensively employed and successfully unveiled the underlying atomic-scale physical mechanisms of these exciting materials. In this talk, I will overview our most recent results on the electronic structure of prototypical structures of layered halide perovskites, vacancy ordered double perovskites, and low dimensional halide perovskite-like materials. I will present the key details of their electronic structure for each type of system that define their experimentally observed optical properties and achieved performances. Our results show how well (or how bad) these different types of materials can perform for different opto-electronic applications ranging from indoors and outdoors PV, light emitters. Furthermore, I will present results the substitutional engineering for the class of halide double salts most promising for low-light PVs. Finally, in the last part of my talk, I will focus on our latest state-of-the-art ab initio calculations of the charge carrier transport properties when comparing three-dimensional ABX<sub>3</sub> and layered halide perovskites. Our results explore directly the effects of structural dimensionality on the carrier mobilities of a selection of prototypical layered perovskites and identify the importance of the intrinsic carrier density in layered compounds to the exhibited transport properties.