**Interaction of MXene and Perovskites**

A. Pecchia, A. Di Vito, D. Rossi, M. Auf der Maur, A. Di Carlo

*Univ. of Rome Tor Vergata, Roma, Italy*

Abstract

MXenes are a relatively recent new family of two-dimensional nanocrystals of transition metal carbides that can be esfoliated from MAX phases. They are typically metallic but depending on the metal ion they can also be semiconducting.

Among the other interesting properties they show a very wide workfunction range, going from 6.0 eV to less than 2.0 eV, depending on the surface terminations. The WF tuning by chemistry opens possible applications in device engineering, since MXene can be placed as interlayer in organic and hybrid devices in order to tune the band-alignment at interfaces.

Indeed MXene show an outstanding ability in improving photovoltaic devices based on Perovskite, where their insertion in low concentration is able to rise the electrical efficiency from 16% to above 20%.

In this work we show DFT calculations of the WF of MXenes and their interaction with Perovskites (MAPbI3). With the help of device simulations we indicate the conclusions that MXene are able to tune the band-alignment at both interfaces with electron and hole transport layers, improving the photocell characteristics.