# Electronic structure of two dimensional titanium carbide multi-layers from valence EELS and *ab initio* calculations: insights into the surface functionalization groups.

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$Ti_3C_2T_2$, where T=OH or F are surface functionalization groups, belongs to the large family of MXene (M being a transition metal and X either C or N) which are few atomic layers thick two-dimensional (2D) transition metal carbide or carbonitride sheets. In the MXenes family, $Ti_3C_2T_2$ is the most studied: it has been shown to exhibit outstanding properties for energy storage applications among others. In this system, the surface groups play a key role: they affect the energy storage capacities or modify their optical properties. Given their crucial role, these functionalization groups have been intensively investigated, but mainly from a theoretical point of view.

In this context, we present a combined experimental and theoretical investigation of the electronic structure of $Ti_3C_2T_2$ based on valence electron energy-loss spectroscopy. Besides evidencing important similarities between the $Ti_3C_2T_2$ and TiC valence electron gases behaviors, a clear interband transition related to the most stable site of the T functionalization groups is identified in the VEEL spectrum. This spectral signature, allowing for the investigation of the T groups at the nanometer scale, is has a prominent effect on the optical properties. In particular, it leads to a 40% variation of the optical conductivity of $Ti_3C_2T_2$ in the middle of the visible energy range which is of major interest for optical or sensing applications.