Towards high-throughput screening of 2D materials for high-power batteries

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MXenes, a large family of two-dimensional transition metal carbides and nitrides, have emerged as promising materials for electrochemical energy storage [1]. Mxenes are usually obtained through the exfoliation of MAX phases and have the generic formula $M_nX_{n+1}T_x$ where M is an early transition metal, X is carbon or nitrogen, and T stands for surface termination(s). The vast chemical diversity of MXenes requires a systematic exploration through automated first-principles calculations and multiscale modeling strategies to identify the most suitable materials for energy storage.

A database of 2,784 MXene structures was explored [2] through the implementation of an automated density functional theory (DFT) workflow to generate input files, optimize structures, evaluate atomic charges... The Bader charge analysis conducted reveal a clear influence of the surface terminations (-O, -OH, -F…) on the Bader charges and volumes. This influence seems to be predominant over the impact of the thickness of the MXene or its carbide or nitride nature. Strong differences between core and surface transition metal atoms are also observed.

An ongoing perspective of these calculations is to provide parameters for classical simulations of MXene based energy storage devices using the constant potential approach [3]. Such simulations would allow one to model operating conditions and charge storage mechanisms at electrode/electrolyte interfaces, an important step for evaluating the electrochemical performance of MXenes.

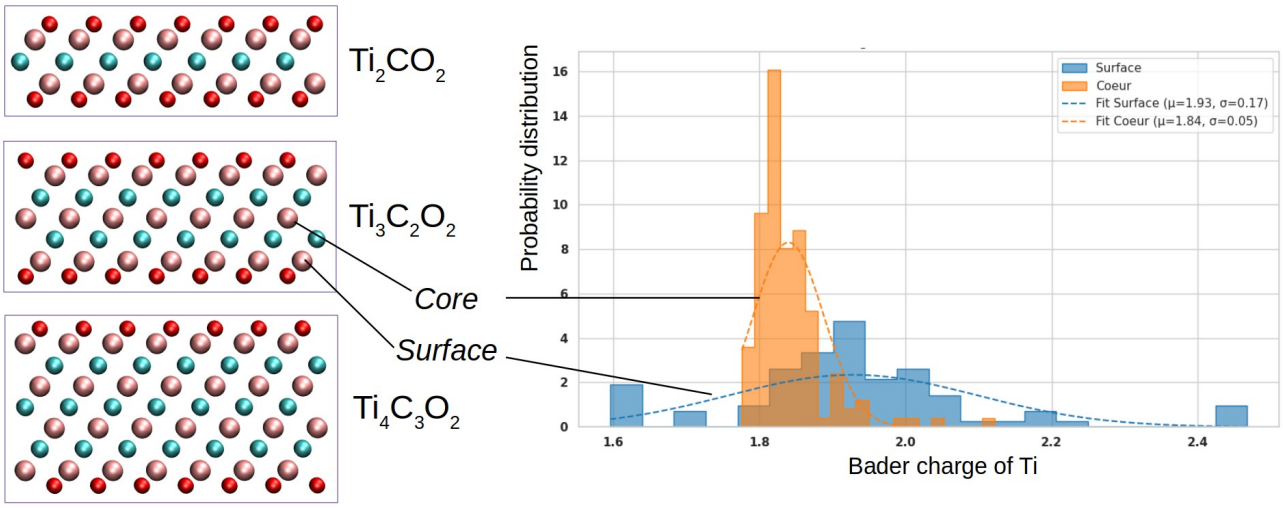

Figure: Example of distributions of Bader charges for Ti atoms in $Ti_nX_{n+1}T_x$ Mxenes.

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