First principle studies of structural and electronic properties of Ti_3C_2 and Ti_2C layered materials crucial for bioactivity of MXenes

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MXenes constitute a new interesting group of 2D materials with an unique biophysical properties [1]. Metal carbides such as Ti_3C_2 and Ti_2C are the main representatives of MXenes materials, very promising to be applicable in biotechnology or nanomedicine. It has been recently shown that these two representatives exhibit different response towards bacteria cells, namely Ti_3C_2 was toxic towards selective bacteria's cells, whereas no such an impact was found in the case of Ti_2C [2]. The understanding of the underlying mechanism of such effect is a fundamental issue for potential development of new generation of drugs. To shed light on this intriguing issue, the *ab initio* calculations in the framework of the density functional theory will be presented for different surface termination (*-F*, *-OH*, *-H*, *-O*) of Ti_3C_2 and Ti_2C structures. The structural and electronic properties will be discussed and compared. All the aspects presented in this communication will be compared with the experimental findings.

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