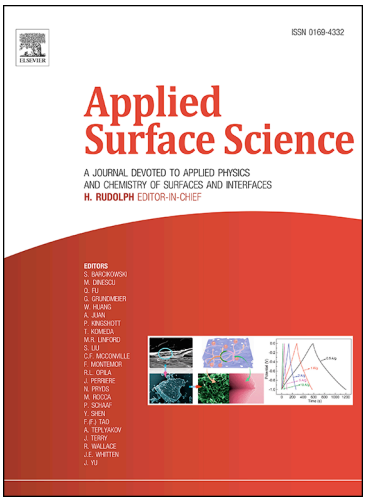

Full Length Article

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PII: S0169-4332(18)32686-2
DOI: https://doi.org/10.1016/j.apsusc.2018.09.254
Reference: APSUSC 40558

To appear in: *Applied Surface Science*

Received Date: 25 June 2018
Revised Date: 27 September 2018
Accepted Date: 28 September 2018

Please cite this article as: Y. Gao, Y. Cao, Y. Gu, H. Zhuo, G. Zhuang, S. Deng, X. Zhong, Z. Wei, J. Chen, Xiang-Pan, J-g. Wang, Functionalization Ti_3C_2 MXene by the Adsorption or Substitution of Single Metal Atom, *Applied Surface Science* (2018), doi: https://doi.org/10.1016/j.apsusc.2018.09.254

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Abstract

Chemical modification of MXenes, as an effective strategy to improve the electronic harmony with other materials, paves huge impetus to their practically industrial application. In this study, by means of Density Functional Theory (DFT) calculations, the adsorption and substitution of single transition metal atoms (M= 3*d* (Fe, Co, Ni, Cu, Zn), 4*d* (Ru, Rh, Pd, Ag, Cd), 5*d* (Os, Ir, Pt, Au, Hg)) on Ti_3C_2 MXene have been systematically investigated. It is found that the adsorption (adsorption energies E_{ad}= -1.05~-7.98 eV) of single metal atoms on Ti_3C_2 are much stronger than those on graphene and graphyne. Interestingly, via a series of electronical structure calculations, we found good linear correlation between E_{ad} and chemically properties (such as the average bond distances $d_{M\text{-}Ti}$, the bader charge and the *d*-electron centre of metal), shedding light on the harmonic effect of doping metals both electronical and geometrically. In other words, the stronger adsorption, shorter bond distance, more bader charge, less negative *d*-electron centre. While for the