

19th World Congress on

Materials Science and Engineering

June 11-13, 2018 | Barcelona, Spain

First-principles study of optoelectronic, transport and ionic sieving properties of $\text{Ti}_3\text{C}_2\text{X}_2$ ($\text{X}=\text{O}$, OH and F) MXene

Golibjon R. Berdiyev, M. Madjet and K. Mahmoud
Hamad bin Khalifa University, Qatar

MXenes, a new family of low-dimensional materials, have received a lot of interest due to their unique physical, chemical, and mechanical properties [1]. MXenes have already shown a great potential in storage applications due to their impressive capacitive performance [2]. Here, we study the electronic and transport properties of Ti_3C_2 MXene using density-functional theory (DFT) in combination with the nonequilibrium Green's function formalism [3, 4]. Fluorinated, oxidized and hydroxylated surfaces are considered. We found that the surface termination has a considerable impact on the electronic transport [3]. For example, the fluorinated sample shows the largest transmission, whereas surface oxidation results in considerable reduction of the electronic transmission. Such enhanced transmission originates from the extended electronic states and smaller variations of the electrostatic potential profile. We also study the effect of lithium and sodium ion adsorption on the electronic transport properties of the MXene [4]. Optical properties of MXene are also affected by surface functionalization [5]. For example, in the visible range of the spectrum, the oxidized sample shows larger absorption, whereas surface fluorination results in weaker absorption as compared to pristine MXene. Recently, MXene nanosheets have also emerged as ultrathin and high-flux sieving membranes [6]. In addition to ultrafast water flux, both hydration radius and charge dependent transport of ions have been observed. MXenes are also shown to be highly resistive to biofouling [7]. Here we present the results of our DFT calculations to explore the possible mechanisms for the charge-selective ionic transport through $\text{Ti}_3\text{C}_2\text{X}_2$ ($\text{X}=\text{O}$, OH or F) MXene [8, 9]. We show that the charge selectivity originates from the charged nature of the MXene layers: the system shows dynamic response to the intercalating ions, even in their hydrated states, by changing the interlayer spacing. We also address the stability of MXene membranes and discuss the possibilities of enhancing their stability by molecular and nanoparticle intercalations. We present the results of our atomistic scale calculations for structural, electronic water sieving properties of hydrophobic graphene and hydrophilic MXene monolayers (see Fig. 1)..

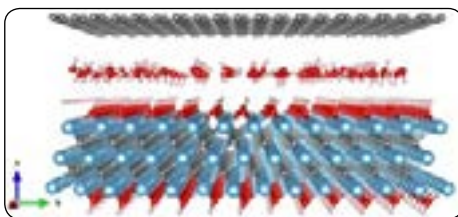


Figure 1: Atomistic structure of graphene (top) and $\text{Ti}_3\text{C}_2(\text{OH})_2$ MXene (bottom) bilayer with intercalating water molecules

Recent Publications:

1. M. Naguib, V. N. Mochalin, M. W. Barsoum, Y. Gogotsi, 25th Anniversary Article: MXenes: A New Family of Two-Dimensional Materials, *Adv. Mater.* 26, 992 (2014).
2. J.-C. Lei, X. Zhang, Z. Zhou, Recent advances in MXene: Preparation, properties, and applications, *Front. Phys.* 10, 276 (2015).
3. G. R. Berdiyev, Effect of surface functionalization on the electronic transport properties of Ti_3C_2 MXene, *Europhys. Lett.* 111, 67002 (2015).
4. G. R. Berdiyev, Effect of lithium and sodium adsorption on the electronic transport properties of Ti_3C_2 MXene, *Appl. Sur. Sci.* 359, 153 (2015).

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5. G. R. Berdiyev, Optical properties of functionalized Ti₃C₂T₂ (T = F, O, OH) MXene: First-principles calculations, AIP Advances 6, 055105 (2016).
6. C. E. Ren, K. B. Hatzell, M. Alhabeb, Z. Ling, K. A. Mahmoud, Yury Gogotsi, Charge- and Size-Selective Ion Sieving Through Ti₃C₂ T x MXene Membranes, J. Phys. Chem. Lett. 6 (2015) 4026-4031.
7. K. Rasool, K. A. Mahmoud, D. J. Johnson, M. Helal, G. R. Berdiyev, and Y. Gogotsi, Efficient Antibacterial Membrane based on Two-Dimensional Ti₃C₂T_x (MXene) Nanosheets, Scientific Reports 7, 1598 (2017).
8. G. R. Berdiyev, M. E. Madjet, and K. A. Mahmoud, Ionic transport through Ti₃C₂(OH)₂ MXene: first principles calculations, Applied Physics Letters 108,113110 (2016).
9. G. R. Berdiyev and K. A. Mahmoud, Effect of surface termination on ion intercalation selectivity of bilayer Ti₃C₂T₂ (T=F, O and OH) Mxene, Applied Surface Sciences 416, 725-730 (2017)..

Biography

Golibjon R. Berdiyev is a Scientist in Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University. He has an experience in performing theoretical investigations on structural, optoelectronic and transport properties of molecular and low-dimensional systems. Currently, he is interested in conducting material science research with a focus on predicting novel materials for photovoltaics, energy storage applications and membranes materials for water treatment. In his studies he mostly uses first principles methods (such as Density Functional theory in combination with the non-equilibrium Green's function formalism) and other atomistic scale methods such as force field based molecular dynamics. He has published more than 100 research articles, which have already received more than 1600 citations. He was awarded for his research including the best research award at University of Antwerp.

gberdiyev@hbku.edu.qa

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