Tnano 2020

International Workshop on Nanotechnology (Tnano20)
October 5 – 8, 2020, in Tbilisi, Republic of Georgia

TWO FACES OF A DOUBLE WELL: MULTIFUNCTIONAL DEVICE BASED ON A TI_2O MONOLAYER AND MAGNETO-MECHANICAL SWITCH BASED ON A MXENE NANOTUBE

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The presentation will consist of two parts. In the first part a new concept of multifunctional nanodevices as potential replacements for common transistors will be presented and a Ti_2O monolayer as an example of such a nanodevice will be discussed. Our study based on density functional theory indicates that a Ti_2O layer is bistable for two lattice parameters, being metallic for one and semiconducting for another parameter. In a switching configuration, this provides a high current ON/OFF ratio when the layer is biased and stretched simultaneously. The high sensitivity of conductance to layer stretching can be utilized for electromechanical switching, the bistability may provide a potential for application as a nonvolatile memory bit, while the current-voltage characteristic of the material in its semiconducting phase indicates a possible use as a varistor. The second part of the presentation will be about structural and magnetic properties of MXene nanotubes. Our density functional theory-based study predicts the existence of two mutually transformable polymorphs of Mo_2C nanotubes with strikingly different properties. One polymorph exhibits unusual negative strain energy with respect to the planar Mo_2C structure and the absence of any long-range magnetic order. The second polymorph displays an antiskyrmionic spin texture with a net magnetization along the tube's axis. The two nanotube polymorphs may be converted into each other by axial tensile or compressive strains, allowing for their application as a magneto-mechanical switch and eventually a nonvolatile magnetic memory unit.

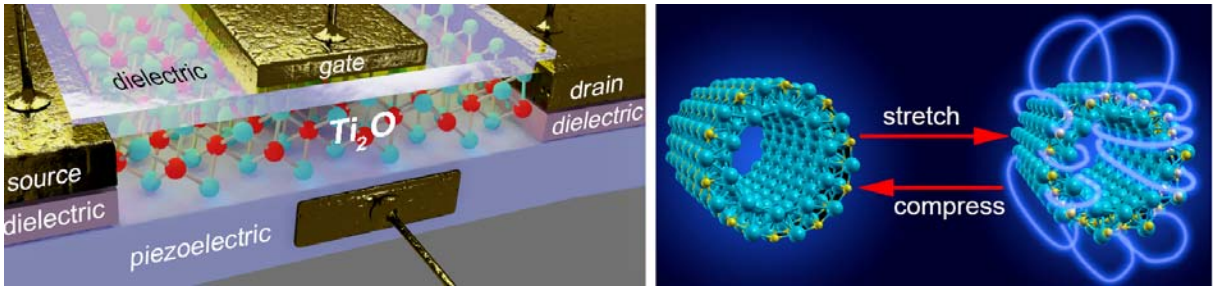

Figure 1. Bistable nanodevices based on layered Ti_2O and MXene nanotubes