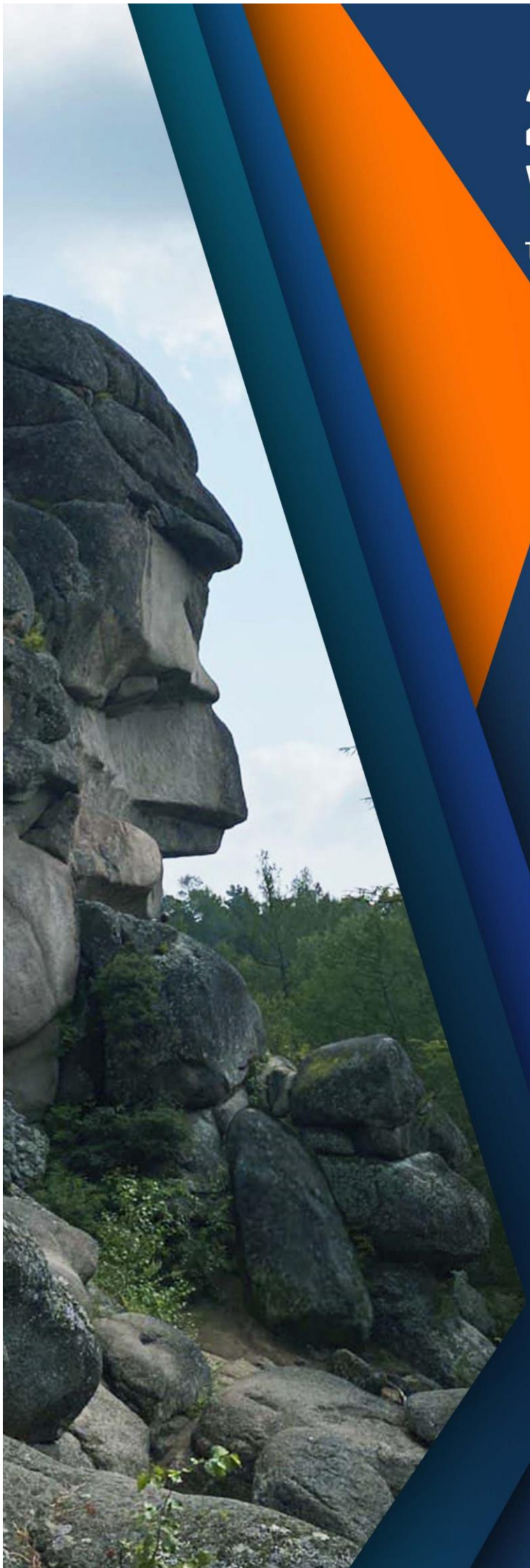

2nd FunMAX WORKSHOP 2021

The second international workshop on the properties of Functional MAX Materials

Book of Abstracts

September 14 - 17, 2021

Kirensky Institute of Physics
Siberian Federal University
Krasnoyarsk, Russia

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2nd FunMAX WORKSHOP 2021

Organized by
Laboratory of Magnetic MAX Materials
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Main topics:

- MAX and MAB phase materials
- Synthesis (bulk, thin films)
- Electrical and thermal transport
- Optical spectroscopy
- Mechanical and chemical properties
- Magnetic MAX phases
- Superconducting MAX phases
- Measurement techniques
- 2D materials: MXenes and similar
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Plenary Lectures

On MXenes and Clays; or What Happens Between the Sheets

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Discovered in 2011, the 2D early transition metal carbides known as MXenes - obtained by etching the A-layers from the MAX phases - have generated substantial interest in the scientific community because of their potential in an ever-expanding host of applications. Whether during etching or use, it is critical to understand what happens in the interlayer space. In most applications, the first step is to etch and wash MXene multilayers, MLs, until they disperse. Using primarily XRD diffraction, the relationships between etchant used and washing protocols and the swelling of the interlayer space of $Ti_3C_2T_x$ MLs is elucidated. How changing the intercalant cations or pH can change the spacing, and even the nature of $Ti_3C_2T_x$ MLs from hydrophilic to hydrophobic, is discussed. How to render MXenes oxidation resistant in aqueous solutions is described. Lastly the close relationship between MXenes and clays are overviewed.

MAX phases and beyond – past, present, and future

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The number of MAX phases have grown significantly since its discovery in 1960 and in the last decade we have seen the realization of its two-dimensional derivative, MXene (1,2). MAX phases and MXenes are versatile in terms of chemical composition, which facilitate controlled and tailored properties. Widening and enhancement of MAX phase and MXene properties requires an enlarged palette of compositions. Since MXenes are derived from MAX phases, the composition of the MAX phase will ultimately affect the resulting MXene. The compositional parameter space of MAX phases is large, and only a small fraction has been experimentally realized. In the quest for a continued expansion of MAX phase compositions different theoretical approaches are used with diverse results. By revisiting the theoretical stability for experimentally known MAX phases it is possible to demonstrate that formation enthalpy is the key for reliable stability predictions.

Alloying by adding a fourth element is one way of expanding the compositional space and, in turn, the attainable properties. This has traditionally been realized through formation of a solid solution upon metal alloying and recently through formation of chemically ordered metal layers (3-5). Theory is powerful for accelerating the exploration of MAX phases and it will be demonstrated how it can be used to identify the most promising novel material candidates for synthesis and how guidelines can be retrieved for which compositions to be expected as chemically ordered or in solid solution. Furthermore, this computational approach can be applied to explore alloying in materials beyond MAX phases and to guide experimental work in the quest for novel materials (6,7).

Acknowledgement
Swedish Research council and the Swedish National Infrastructure for Computing (SNIC)

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Magnets for energy conversion - state of the art

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High performance permanent magnets are key components of energy-related technologies, such as direct drive wind turbines and e-mobility. They are also important in robotics and automatization, sensors, actuators, and information technology. The magnetocaloric effect (MCE) is the key for new and disruptive solid state-based refrigeration. Magnetic hysteresis – and its inherent energy product - characterises the performance of all magnetic materials. Despite considerable progress in the modelling, characterisation and synthesis of magnetic materials, hysteresis is a long-studied phenomenon that is still far from being completely understood. Discrepancies between intrinsic and extrinsic magnetic properties remain an open challenge and magnets do not operate yet at their physical limits.

Basic material requirements, figure of merits, demand and supply, criticality of strategic elements are explained for both permanent magnets and magnetocalorics. Benchmark materials like NdFeB and LaFeSi are described in order to rank possible alternative material classes like the MAX-phases.

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Expanding the structural and elemental space of MAX phases and MXenes – from carbides to borides

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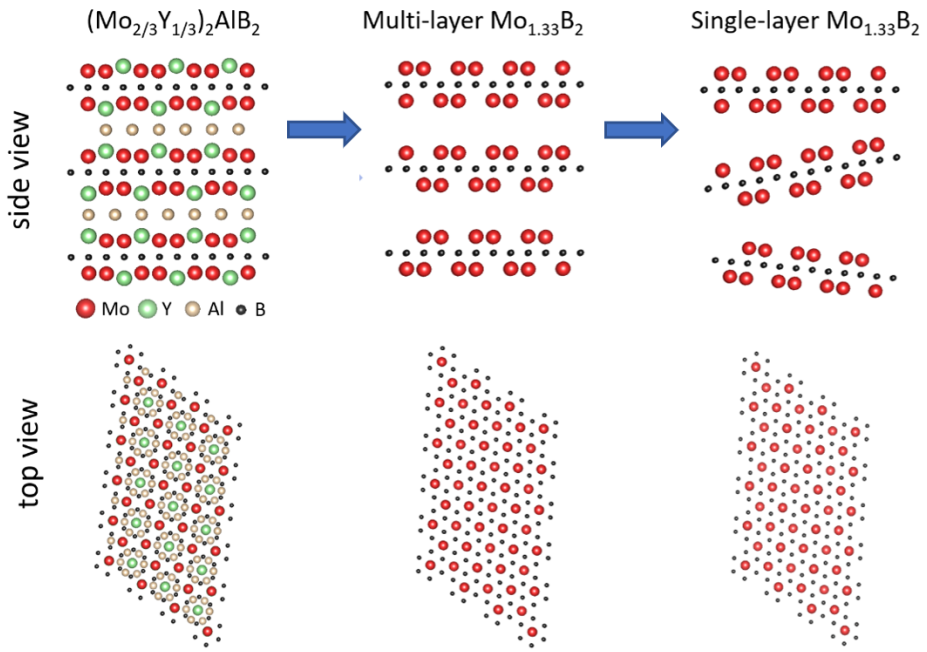
The exploration of laminated metal carbides and nitrides in the form of MAX phases and MXenes is an area of materials discoveries. A more recent addition to the field is a new type of atomic laminated phases, coined *i*-MAX, in which the M-atoms in $(M1_{2/3}M2_{1/3})_2AlC$ are in-plane chemically ordered. The first phase discovered was $(Mo_{2/3}Sc_{1/3})_2AlC$, and it has been shown that this was a first example of a large, more than 30 reported to date, set of thermodynamically stable phases, typically obtained from an interplay between theoretical predictions and experimental verification. The *i*-MAX phases realize 3D and 2D materials with elements beyond those traditionally associated with MAX phases and MXenes, and expand the range of attainable properties. The present talk will summarise the current state of *i*-MAX and *i*-MXene synthesis, and how the knowledge and understanding of these materials can be transferred from atomically laminated carbides to corresponding borides. This has implications for the tuning potential in applications for, e.g., energy storage and catalysis. The 3D to 2D conversion of a laminated boride is shown in the image below.



MAX phase electronic properties measured from single crystals

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The availability of single crystals is key for a better understanding of any electronic or other physical property of MAX phases. We shall present a collection of results issued from single crystal experiments mainly conducted on large scale instruments. We will show how these results, when combined with theory and *ab initio* calculations, do not only shed light on some specific aspects, but also allow one to draw general and unifying considerations about the physics of MAX phases.

Invited talks

Synthesis of new compositions and morphologies of MAX phases

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We are facing many exciting challenges in materials science and being able to produce high-quality and new materials plays a key role in unraveling the almost endless list of open research questions and developing new technologies. My group focuses on the synthesis of new layered compounds (MAX phases) and 2D materials. Traditionally, they are prepared by high-temperature solid-state methods, oftentimes under pressure, and the formation of side phases (binary carbides/nitrides and intermetallics) is very common and a challenge in the materials science community. In this talk, I will show wet chemistry-based synthesis strategies to access MAX phases that lead to new members as well as novel microstructures of these types of materials. For example, we have synthesized thick films, (hollow) microspheres and microwires of MAX phase Cr_2GaC. Besides, we also push towards nitrides and carbonitrides and have prepared some hitherto unknown compositions. We study the materials´ (local) structures by X-ray and neutron diffraction and focus on their complex and unique transport properties.

We gratefully acknowledge support by the ACS through a Petroleum Research Fund award number AWD34170 as well as funding from the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 405553726 – TRR 270.

Spin Resolved Analysis for Angular Resolved Photoemission Spectroscopy and Momentum Microscopy

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Spin and momentum-resolved measurements are experiencing increasing importance for modern surface analysis. Several ways exist to determine the spin within the framework of photoemission spectroscopy. We present three technologies to study the electron spin for state-of-the-art ARPES instruments and modern momentum microscopes. ARPES instruments, providing an energy dispersive image of the angular electron emission distribution, can be equipped with combined 2D detectors and a three-dimensional single line spin detector. The unique combination of a 90° deflector and a highly precise magnetic spin rotation lens allows to study all three spin components on one spin detector of either Mott or VLEED type. Momentum Microscopes, showing k-space resolved constant energy maps, can additionally be operated with a novel imaging type detector, the direct imaging (DI) spin detector, based on spin orbit interaction on an iridium target. The use of the magnetic spin rotator lens allows a stable operation at optimal scattering energy and allows to measure 2 in plane spin components when switching between the spin rotator mode and the scattering energy mode.

Elemental mapping and imaging of magnetization and its dynamics on the micro- and nanoscale by Scanning Transmission X-ray Microscopy

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Magnetic materials on the micro- and nanoscale are addressing a wide spectrum of contemporary challenges ranging from cancer research towards spintronic and magnonic solutions for modern information technology [1-3]. Magnetic MAX phases are projected as a well suited class of materials for the development of latter applications [4] with their two-dimensional representations called MXenes offering an intriguing potential in spin based computing due to their rich electronic and magnetic tunability by surface functionalization [5]. The synchrotron-based technique of Scanning Transmission X-ray Microscopy (STXM) allows the element-specific and spatially resolved ($\geq$ 10 nm [6]) chemical and magnetic characterization of such materials in a wide range of X-ray absorption energies. By exploiting X- ray Magnetic Circular Dichroism (XMCD), information on orientation and size of magnetic moments can be determined, probing the sample by circularly polarized X-rays at a photon energy set to an X-ray absorption edge of the investigated element [7]. Time-resolved STXM (TR-STXM) allows to monitor dynamic excitations of the magnetization up to 10 GHz with $<$ 30 ps sampling [8]. The talk will introduce Scanning Transmission X-Ray Microscopy, XMCD and the sum rules, with the focus on time-resolved STXM and its application to element-specifically detect magnetization dynamics on the micro- and nanometer scale. Exemplary measurements demonstrate elemental mapping of RE-i-MAX (RE = Tb, Gd) [9] by STXM and the TR-STXM based imaging of uniform and non-uniform resonant responses in Py/Co bilayer, and Py stripe [10] microstructures and Fe_3O_4 nanoparticles chains within magnetotactic bacteria *Magnetospirillum Magnetotacticum* [11].

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Prospects and challenges for bioactivity and toxicity of the MXenes

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The past few years have witnessed significant development in the chemistry and potential biological applications of two-dimensional (2D) materials. Innovative 2D carbides, nitrides and carbonitrides of early transition metals, called MXenes, have been also extensively studied for several years on the applications in human health protection. It is currently accepted that the specific functionalities of the MXenes can result in wide spectrum of bio-activities. In this context, MXenes are currently being carefully studied, with strong attention to mechanisms of action and biocompatibility features. We already know that MXenes exhibit different cellular effects which can be additionally induced by multiple external or internal factors. These effects are in turn strictly dependent on MXenes structure, chemical composition, and surface characteristics which positively support their interesting potential in nano-therapies.

In fact, MXenes are promising anticancer agents, which can not only inhibit proliferation of cancer cells but also induce oxidative stress, and even influence the cell functioning and cell cycle through inducing programmed cellular death (apoptosis). On the other hand, such a wide range of bio-activities may inevitably cause unexpected toxicological effects that require a broader understanding. The obtained results clearly indicate that in this respect, the surface chemistry of MXenes has a significant impact on their biological properties. This is closely related to the synthesis methods and also oxidizing properties, leading to the occurrence of potentially toxic superficial metal oxides.

In the case of MXenes, the challenge now relates not only to obtain the needed biological properties but above all, to understand and maintain (stabilize) them in the desired environment. The presented studies will shed some light on the issues raised above and also outline new directions in toxicology of the MXene phases. They are focused on elucidating antiproliferative, pro-oxidative, and pro-apoptotic mechanisms of action.

The presented results were accomplished thanks to the subvention funds allotted by the National Science Centre, within the framework of the research project ‘SONATA BIS 7’ no. UMO-2017/26/E/ST8/01073.

Features of MagMAX thin film deposition techniques

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The structural features that distinguish magnetic nanolayers from bulk isotropic systems impose significant difficulties in their synthesis. The requirements for high purity of the used reagents and the presence of an ultrahigh vacuum in the technological chamber are usual. There are also high requirements for the surface sensitivity of analytical methods for such systems. It is also advisable to analyze samples under ultrahigh vacuum conditions without exposing them to air, i.e. in situ mode.

In this regard, we use a custom-made sputtering complex for the synthesis of magnetic MAX phases. The achievable base pressure is 10^{-9} Torr. The complex contains a load-lock for clean cassette loading of samples. Residual gases are monitored by a mass spectrometer. An Ar-ion gun and a combined HEED, LEED and AES system are integrated into the main process chamber. An optical system for in situ measurement of magnetic susceptibility based on MOKE is provided.

The potential technological capabilities of the complex allow either simultaneous deposition of up to four materials (including dielectric materials) from magnetron sources, or sequential sub-nanometer layers from up to four PLD targets. The sample temperature is provided by a molybdenum substrate holder ranging from 100 to 1200 K with a gradient of less than 20 K per cm. Heating of the substrate holder by an electron beam.

The results of the first experiments on the synthesis of test samples from magnetron sources are shown. And also the results of PLD tests for Mn, Fe, Ge, Si and C are discussed.

Acknowledgement
The research was supported by the government of the Russian Federation (agreement No. 075-15-2019-1886).

Effect of Interfaces in the Multilayer Structures on the Electronic States

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All elements of dielectric permittivity tensor for multilayer structure with magnetic layer can be found by magnetoellipsometry measurements. Recently we have found that in the $Fe/SiO_2/Si$ structure the elements of dielectric permittivity tensor of the Fe layer deviate from ist bulk values for the Fe layer thikness d_{Fe} 77nm and less [1]. Moreover, for the d_{Fe} 11nm the effect of interfaces vacuum/Fe and Fe/SiO_2 appears to be quite important. Two reasons may induce the interface effect, the reconstruction of the electronic structure or the reconstruction the dipole matrix elements. Assuming the dipole matrix elements weakly dependent on the wave number over the Brillouin zone we have write down the general RPA expression for the elements of dielectric permittivity tensor as a product of the interband density of states and the average matrix elements. In this representation the ratio Im $\varepsilon_{xx}(\omega)$/ Im $\varepsilon_{xy}(\omega)$ is expected to be energy independent. We have verify this prediction experimentally.

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Two-dimensional Molybdenum Carbide MXenes for highly sensitive hygrometer sensors

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MXenes, two-dimensional (2D) transition metal carbides or nitrides, have recently shown huge potential for gas sensing applications [1,2]. We have successfully synthesized 2D Mo_2CT_x flakes via selective chemical etching of Ga from the Mo_2Ga_2C precursor. The comprehensive characterization of the MXene by XRD, SEM, TEM, AFM, and XPS shows high quality flakes with lateral dimensions of 0.5-1 μm. Delaminated Mo_2CT_x MXenes were deposited on a multi-contact array to study their chemiresistive performance for organic vapors (methanol, ethanol, n-butanol, acetone, ammonia) and humidity at 10^1-10^4 ppm concentrations in dry air. We demonstrate that Mo_2CT_x MXenes are highly sensitive towards H_2O vapor in comparison to the organic analytes showing a dc chemiresistive response at a 10 ppm detection limit. Moreover, humidity suppresses the response of Mo_2CT_x to organic analytes due to the blocking of active sites.

In addition to their high sensitivity, Mo_2CT_x MXenes enable a selective recognition of analytes, such as low molecular weight alcohols, as shown by linear discriminant analysis. By measuring the impedance of MXene layers as a function of ac frequency in the 10^{-2}-10^6 Hz range, we demonstrate that the sensor array changes resistance rather than capacitance. The sensor transfer function allows us to conclude that the Mo_2CT_x chemiresistance is mainly originating from electron transport through inter-flake potential barriers with heights up to 0.2 eV. DFT calculations, describing the Mo_2C surface interaction with organic analytes and H_2O, fully explain the experimental data as a shift of electron density under the analyte's adsorption which increases electrical resistance [3]. We suggest that the observed performance of Mo_2CT_x in dry air meets many sensing applications in hygrometry at ultra-high sensitivity and opens avenues for implementation of new 2D concepts in practice.

Acknowledgement

This work has been partially funded through the project EUROFEL-ROADMAP ESFRI. D.A.K. thanks RFBR, project no. 19-32-90160, for the partial support of the DFT calculations. This work was supported by the Deutsche Forschungsgemeinschaft (DFG) within CRC/TRR 270, project B02 (Project-ID 405553726).

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Predicting exfoliability of MXenes using high-throughput *ab initio* reaction thermodynamics

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MXenes are typically synthesised by selective removal of the 'A' element from precursor MAX phases in an etching environment. Despite the large number of known MAX phases, this approach has currently enabled the synthesis of only about 30 different MXenes out of which few are solid-solutions, and in-plane/out-of-plane ordered structures [1]. *Ab initio* density functional theory (DFT) calculations may help in guiding experiments to identify further possible MXenes. Predicting exfoliability on the basis of formation energies relative to the elements has proven to be problematic [2]. In this contribution we show that explicitly accounting for the etching environment within an *ab initio* reaction-thermodynamics framework is a promising tool for identifying MAX-to-MXene exfoliation routes [3]. Thereby, the reaction energy of MXene formation is determined in comparison to other possible competitive reactions, acting as the indicator of an (un)feasible exfoliation. Various benchmarks are reported giving confidence in the method. Moreover we report on high-throughput DFT screening of more than 1600 potential MAX phases ($M_{n+1}AX_n$, n=1,2,3, M=transition metal, A=group III & IV element, X=C,N) that may be suited for exfoliation . The method adopted for screening, considers formation energies relative to all possible side phases. Our calculations suggest various new stable MAX phases that have not yet been synthesised and may expand on novel MXenes.

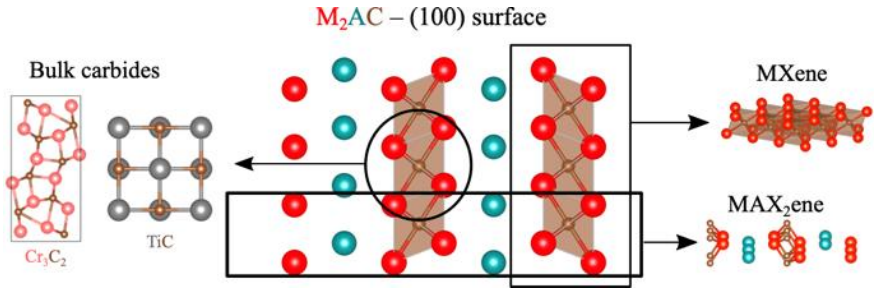

Figure 1. Exfoliability of MXenes is predicted by means of ab initio reaction thermodynamics where various possible reaction pathways in an etching environment are compared

Keywords: High-throughput DFT, MAX phases, MXenes, reaction thermodynamics

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Pulsed Laser Deposition of Epitaxial Cr_2AlC and $(Cr_{1-x}Fe_x)_2AlC$ MAX Phase Thin Films

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MAX phases ($M_{n+1}AX_n$) are ternary or quaternary compounds of layered hexagonal structures, where M is an early transition metal, A is an A group element and X is either C or N [1]. Within the last years, much attention has been put on magnetic MAX phases with Cr and/or Mn as two possible M elements. The magnetic properties of $(M1_{1-x}M2_x)_2AX$ phases are driven by competing ferromagnetic and antiferromagnetic correlations leading to complicated phase diagrams [2-5]. One parent compound of such MAX phases is the Cr_2AlC system which can be doped by a second M element like Mn or Fe.

We grow epitaxial Cr_2AlC and $(Cr_{1-x}Fe_x)_2AlC$ MAX phase thin films on MgO(111) and Al_2O_3(0001) substrates by pulsed laser deposition (PLD) at 600°C with thicknesses of 10-50 nm [6]. The used KrF Laser (248 nm) hits elemental targets at an energy density of 13 J cm^{-2}. For Cr_2AlC thin films on MgO (111), X-ray diffraction and morphology studies reveal phase purity, columnar growth, the epitaxial relation $Cr_2AlC(0001)$ || MgO(111) and Cr_2AlC [11-20] || MgO[10-1] and similar growth modes on Al_2O_3(0001). Resistivity measurements show semiconductor-like behaviour for 10 and 20 nm thick films, and metallic-like behaviour for thicker films, suggesting a percolation thickness slightly above 20 nm. Our results demonstrate the potential of PLD as a novel method for the growth of epitaxial MAX phase thin films.

In a second series, we grow $(Cr_{1-x}Fe_x)_2AlC$ MAX phase thin films with $0 < x < 0.2$ by PLD at 600°C and obtain similar growth modes on MgO(111) and Al_2O_3(0001) as for the Cr_2AlC parent compound [7]. However, X-ray Diffraction and Transmission Electron Microscopy reveal a coexisting $(Fe,Cr)_5Al_8$ intermetallic secondary phase. Our experiments suggest an actual maximum Fe solubility of 3.4 at%, corresponding to $(Cr_{0.932}Fe_{0.068})_2AlC$, which is the highest value of Fe doping reported up to now in volume materials and thin films. Residual Fe is continuously distributed in the $(Fe,Cr)_5Al_8$ intermetallic secondary phase. The incorporation of Fe results in the slight reduction of the *c* lattice parameter while the *a* lattice parameter remains unchanged. These findings are fully supported by Density Functional Theory predicting phase stability for $0 < x < 0.2$.

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Magnetic, electronic, optical and elastic properties of magnetic $(Mn_xFe_{1-x})_2(Ga_yAl_{1-y})C$ MAX phases

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The investigation and discover of new functional magnetic materials with the prospective properties are ones of the primary tasks of physics and chemistry. The magnetic MAX phases are ones of such materials. The addition of new combinations of elements in the MAX phases allow the properties of functional materials to be tuned. In the present work the magnetic, electronic, optical and elastic properties of $(Mn_xFe_{1-x})_2(Ga_yAl_{1-y})C$ phases (x, y=0..1) were studied within DFT-GGA.

An ab initio study of extreme cases at x, y = 0 and 1 have been revealed that Mn_2GaC and Mn_2AlC are ferromagnets (FM), while the iron-based compounds Fe_2GaC and Fe_2AlC are antiferromagnetic (AFM). Further research have predicted $(Mn_xFe_{1-x})_2(Ga_yAl_{1-y})C$ as a new magnetic nanoscale laminate, with a FM of AFM state dependent on the Mn-Fe atomic configuration on the M site of MAX phase. FM state is favorable for $(Mn_xFe_{1-x})_2GaC$ and $(Mn_xFe_{1-x})_2AlC$ with x >0.875 (Table1) and x>0.75, correspondingly. The study of phase stability of M_2AX phases was performed using DFT calculations of the MAX phase's formation enthalpy in comparison with the set of competitive phases from ternary phase diagrams by combination with linear optimization procedures [1]. To date, the authors have not find data on the synthesis $(Mn_xFe_{1-x})_2GaC$ MAX phases, but present analysis of phase stability of these compounds shows, that they are thermodynamically stable with x = 0.875 and 1 only. Table 1 show the total energies (per formula unit) of the MAX phase (E_{MAX}), formation enthalpies of MAX phase (ΔH_{cp}) in comparison of the competitive phases for $(Mn_xFe_{1-x})_2GaC$. At negative ΔH_{cp} compound is considered as stable. Therefore, by replacing the manganese atom with iron, it is possible to obtain a stable antiferromagnetic $(Mn_{0.875}Fe_{0.125})_2GaC$. As for $(Mn_xFe_{1-x})_2AlC$ compounds, they are metastable and could be stabilized be pressures up to 5GPa. To investigate the effect of the A-element on the thermodynamically stability, $Mn(Ga_yAl_{1-y})C$ compounds with Ga incorporation have been studied. The results indicate thermodynamically stability over the composition range y= 0.0 to 0.5 for Ga. These data could motivate experimental investigations on stability of $(Mn_xFe_{1-x})_2(Ga_yAl_{1-y})C$ upon substitution of Mn by Fe and Al by Ga.

Table 1. Ground state, the total energies (per formula unit) of the MAX phase (E_{MAX}), formation enthalpies of MAX phase (ΔH_{cp}) in comparison of the competitive phases for $(Mn_xFe_{1-x})_2GaC$

compound	x	Ground state	E_{MAX}	ΔH_{cp}, eV/atom
$(Mn_xFe_{1-x})_2GaC$	0.000	AFM	-28.76	0.06
	0.250	AFM	-29.26	0.04
	0.500	AFM	-29.78	0.01
	0.750	AFM	-30.23	0.00
	0.875	AFM	-30.47	**-0.01**
	1.000	FM	-30.72	**-0.15**

Acknowledgement. The reported study was funded by Russian Foundation for Basic Research, Government of Krasnoyarsk Territory, Krasnoyarsk Regional Fund of Science to the research project № 20-42-240004

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Contributed talks

Investigation of the properties of thin magnetic films

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Studies of the features of the nonequilibrium critical behavior of multilayer magnetic structures can serve as the basis for a better interpretation of experimental data [1]. There is an impressive number of articles aimed at investigating the occurrence of the effects of aging in various materials [2]. The effects of aging are characterized by a slowdown in correlation and relaxation processes with an increase in the "age" of the system, as the time between preparation and the beginning of measuring the characteristics of the sample [3].

This paper presents the results of a Monte Carlo study of the nonequilibrium behavior of the magnetic multilayer Co / Cu / Co structure during the slow evolution of the system from the nonequilibrium initial state for film thicknesses N = 7; 9 monolayers and linear system size L = 128. The calculations were carried out from the high-temperature initial state of the system to obtain the dependence of the autocorrelation function C (t, t_W) on the waiting times, where t_W is the waiting time, t is the observation time.

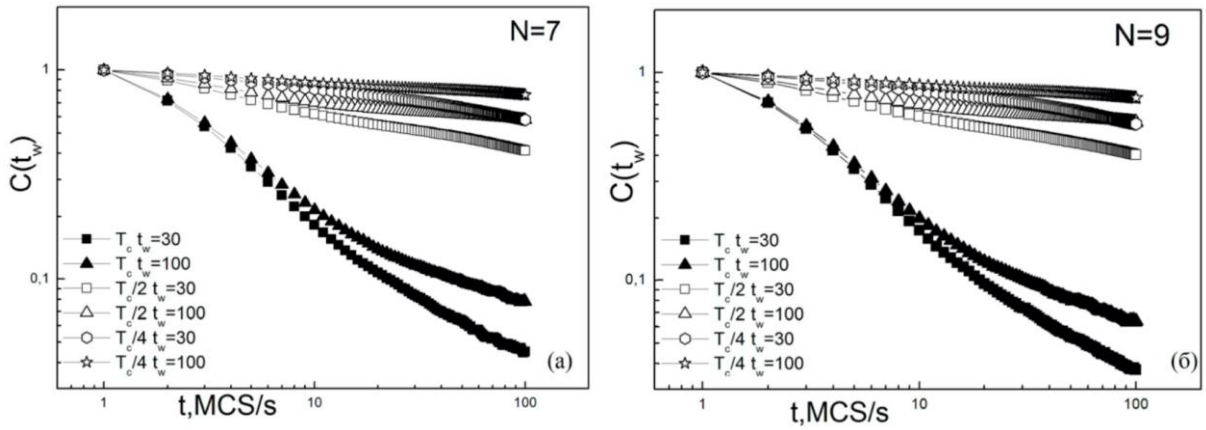

Figure 1 - Dependence C (t, t_W) at t_W = 30; 50; 100 at N = 7 (a) and N = 9 (b). The measurements were carried out at the critical temperature T_C and at 1/2 of T_C.

The appearance of the effects of aging of the autocorrelation function was found, i.e. dependence of the time decay of the correlation effects on the waiting time t_W. The revealed effects of aging for our model of a multilayer structure were obtained in good agreement with the experimental results presented in [4].

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Photocatalytic properties of MXenes stabilized with L-ascorbic acid (Vit. C) in organic dyes degradation

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Scientists prepared many variants of two-dimensional (2D) nanomaterials with unique properties such as high surface area to volume ratio, surface charge design, anisotropic nature, as well as tunable functionalities. Therefore, they have found a wide range of applications in diverse research areas, such as material science, environmental engineering, and protecting the environment due to their catalytical properties [1]. One of them is a novel group of 2D layered transition metal carbides called MXenes. MXenes are characterized with the formula $M_{n+1A}X_n$, where M is a transition metal, A is an A group element, X is a carbon or/and nitrogen, while n = 1–3 or even 4. It is a sandwiched-like structure, composed of layers within octahedral $M_{n+1}X_n$ nitrides and carbonitrides, prepared from MAX phases [2].

Scientists have currently found that MXenes while being relatively unstable, should be modified to increase their properties and efficiency of photocatalysis [3]. However, we were interested in checking the catalytic activity of bare 2D Ti_3C_2 MXene after delamination. For this purpose, we stabilized MXene with L-ascorbic acid (vitamin C). Our work has shown high photocatalytic properties of bare MXenes without the need for any post-processing and surface modification with other compounds supporting the process. The catalyst has been analyzed in terms of specific surface area, colloidal properties, morphology analysis, pore structure of grains, and analysis of light absorption. The photocatalytical properties were also determined by a bandgap. MXene has been used as a photocatalyst to degrade methylene blue using simulated daylight and UV light as well as at eight different wavelengths to verify what energy source is the most effective for the process. Such procedure allowed to increase process- and cost-efficiency. In addition, the catalyst was regenerated and successfully reused. Our research confirmed that the stabilization of MXene by natural antioxidants is beneficial in preserving its catalytic efficiency in degradation of dye pollutants.

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Catalytic properties of MAX phases in selective oxidation reactions

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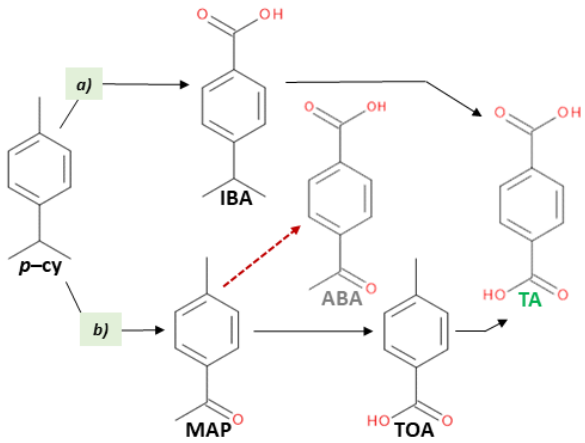
A focused research in the last decades showed that the scientific community handled an important challenge to identify the next generation of sustainable, cost-effective and energy efficient catalytic materials.[1] Selective oxidation reactions of hydrocarbons continue to be in the spotlight of both academia and industry[2] and play a key role for the production of valuable compounds[3] used in important fields, ranging from polymer synthesis to medicinal chemistry.[4]

In this line, selective oxidation of *p*-cymene is an important green industrial chemical process due to the fact that represent a viable alternative to the oxidation of *p*-xylene and valuable products can be obtained, such as terephthalic acid (TA), one of the monomers used for the production of polyethylene terephthalate (PET).[5] Moreover, other reaction products, such as *p*-methylacetophenone (MAP), *p*-toluic acid (TOA) and *p*-isopropylbenzoic acid (IBA) have applications in various fields.[6]



In this study, the catalytic properties of different MAX phases (Ti_3AlC_2, Ti_2AlC, V_2AlC, Ti_3SiC_2, Mo_2Ga_2C and $Mo_2Ti_2AlC_3$) were investigated in catalytic oxidation reaction of *p*-cymene (see Scheme 1), but remarkable results were obtained only in the case of Ti_3AlC_2, Ti_2AlC and Ti_3SiC_2, respectively. With the MAX phase attending as catalyst, the selective oxidation occurred at the methyl substituent as well as at the isopropyl substituent through two different reaction pathways (Scheme 1, a) and b)), generating several reaction products, identified by ^{1}H–RMN.

In conclusion, MAX phases present good activity in p-cymene oxidation reaction, and moreover certain MAX phase compositions are also stable in the reaction conditions used.

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The effect of composition and pressure on phase stability and properties of magnetic M_2AX (M = Mn, Fe; A=Al, Ga, Si, Ge; X=C, N) phases

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The investigation and discover of new functional magnetic materials with the prospective properties are ones of the primary tasks of physics and chemistry. The magnetic MAX phases are ones of such materials. The magnetic properties of M_2AX (M=Mn, Fe; A=Al, Ga, Si, Ge; X=C, N) phases were studied within DFT-GGA. The magnetic electronic ground state is determined. The investigation of phase stability of M_2AX phases is performed by comparing the total energy of MAX phases to that of the set of competitive phases for calculation of the phase formation enthalpy [1]. As the result of such an approach, we have found two stable compounds and six metastable ones (Figure 1). It is shown that several metastable MAX phases (Mn_2AlC, Fe_2GaC, and Mn_2GeN) become stable at an applied pressure of about 5 GPa. One of the predicted stable compounds, namely, Mn_2GeC has not been observed experimentally yet. The mechanical, electronic, elastic, and optical properties of predicted stable and metastable phases are studied.

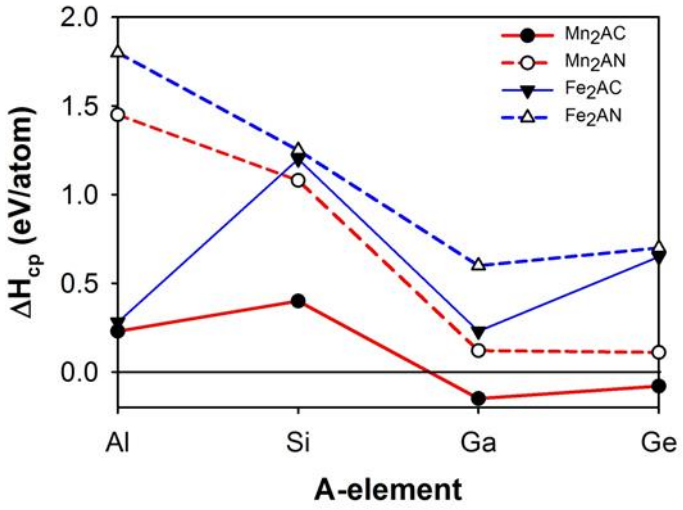

Figure 1. Calculated formation enthalpies of M_2AX phases with respect to most competing phases in dependence on the composition of M-, A- and X-sites.

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On the Magnetoelectric Coupling in $Ni_{(1-x)}Cu_xB_2O_4$

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The mechanism of the magnetoelectric coupling of spins of Ni^{2+} and Cu^{2+} ions with the applied electric field in $(Ni, Cu)B_2O_4$, caused by the coupling of 3*d* electrons with the electric field and by the spin–orbit coupling, is analyzed. It is shown that the ordering of spins in the *ab* crystallographic plane of the crystal induces the electric polarization along the *c* axis of the crystal, and this polarization is mainly related to nickel ions.

To obtain the electric polarization in the CuB_2O_4 antiferromagnet, it turns out to be necessary to apply the magnetic field in the *ab* plane. The dynamical magnetoelectric coupling is also discussed in context with available experimental data for CuB_2O_4.

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Antimicrobial performance of Ti_3C_3 MXene-based point-of-use water filters

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MXenes were first introduced by Naguib *et al.* in 2011. These are transitional metal carbides and/or nitrides, which possess layered structure and unique properties. The most common method of obtaining MXenes comprise selective acid etching of parental MAX phases with the general formula of $M_{n+1}AX_n$. Herein, M stands for a transitional metal, A is an A-group element, X is carbon and/or nitrogen, while n = 1, 2 or 3 [1]. After etching, the obtained $M_{n+1}X_n$ MXene is further delaminated to individual flakes with a wide range of applications [2].

Due to their adsorptive, antibacterial, and hydrophilic properties, MXenes are considered a strong candidate for water treatment applications [3]. In our studies, we have developed Ti_3C_2/Al_2O_3/Ag/Cu nanocomposite-based polypropylene fabrics for potential point-of-use (POU) water treatment solid-bed systems. Due to the poor sanitation conditions, POU solutions need to overcome extraordinary issues such as sufficient efficiency at a high flow velocity, low cost, minimal maintenance, and a long life cycle. As we have proven, after oxidation of polypropylene fabrics modified with Ti_3C_2 MXene and noble metal nanoparticles, it was possible to eliminate microbiological contamination of potentially pathogenic bacteria (*E. coli* and *S. aureus*) from filtered water, despite a noticeable increase in flow velocity. Such effect was not observed in the case of filters modified with pristine nanocomposite. What is more, aged nanocomposite-based filtration material shown "self-disinfecting" properties, as it was able to eliminate more than 99% of adsorbed bacteria cells within 24 hours of contact time at room temperature. Lastly, DLS and zeta potential analysis confirmed the stability of filters, as there was no secondary release of nanocomposite into the filtrate. This work sheds more light on the potential application of MXenes for water treatment as well as on their antibacterial properties and the possibility of functionalization.

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Correlative Raman spectroscopy and EBSD for orientation and strain state analysis in MAX phases

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MAX phases are a highly anisotropic material, giving rise to a large variation in their properties depending on orientation of the crystal lattice. Typically, orientation can be determined through Electron Backscatter Diffraction (EBSD), is a powerful technique with very high spatial resolution and the ability to determine strain in a crystal structure. However, it requires a high level of sample finish, long scan times and can be limited but sample size dependant on the machine used. Raman spectroscopy is highly sensitive to the anisotropic nature of the MAX phases, leading to significant changes to full width half maximums and intensities of peaks. Raman has a lower spatial resolution (~700 nm), but requires essentially no sample preparation and allows for rapid acquisition of data in comparison to EBSD. Therefore, we have been able to correlate orientations provided by EBSD to Raman spectra taken in those grains, allowing for rapid orientation analysis of samples.

As Raman is sensitive to changes in bond length, it can analyse strain at the bonding level, as any change in bond length will lead to a shift in the Raman peak. This makes it an incredibly powerful technique for MAX phases as peaks relating to the M-A and M-X are segregated into two different regions of the Raman spectra. This means it is possible to determine how strain is being accumulated in the different layers of the MAX phase. As each peak shows a specific shift, dependant on orientation and loading orientation, correlating to a specific strain. Therefore, we can determine the extent of the non-homogeneous deformation of the MAX phase lattice through Raman spectroscopy.

Magneto-optical properties of MAX-materials from magneto-optical ellipsometry data

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The method of magneto-optical ellipsometry (ME) is widely used and is very convenient for monitoring the optical, structural, magnetic, magneto-optical properties of synthesized materials. That is why, it is of interest to extend its application to the study of MAX-phases [1], both *in situ* (during the synthesis), and *ex situ* (after the synthesis, outside the vacuum chamber).

We are highly experienced in the ME study of optically isotropic media, we developed and implemented a set of data processing algorithms [2-5]. However MAX-phases quite often are structures with uniaxial anisotropy, that is why we had to develop an algorithm for processing data from anisotropic structures, i.e. to solve the inverse ME problem for optically anisotropic uniaxial structures [6].

It is the taking into account of the magneto-optical response that we need to add to the expressions already known in the literature for the reflection coefficients of anisotropic media [7], connect them with the parameters measured during the ME experiment, and determine expressions for obtaining information about the complex magneto-optical parameter *Q* [7] and about the total dielectric permittivity tensor.

Overall, expressions have been obtained for the reflection coefficients for p- and s-polarization for the interface between the external medium and an optically anisotropic uniaxial sample, taking into account the magneto-optical response in the geometry of the transverse magneto-optical Kerr effect. It was shown how to obtain the magneto-optical parameter *Q* analytically for the chosen geometry of the ME experiment. A scheme for carrying out ME measurements has been developed to obtain all components of the dielectric permittivity tensor of a uniaxial anisotropic material, for example, MAX-phases.

Acknowledgement

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Non-conventional techniques to enhance the doping level in quaternary $(Cr_{1-x}Mn_x)_2AlC$ MAX-phase

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MAX-phases attract the increasing attention due to the unique set of properties, combining metallic and ceramic ones, such as high electric and thermal conductance, elastic stiffness, easy machinability, tolerance to high-temperature corrosion and harsh environments [1]. Thus, MAX-phases are being considered for the number of practical applications, from chemically stable electrical contacts to protective and shielding coatings and high-temperature applications [2]. One intriguing feature is the ability to finely control the physical characteristics of the MAX-phases via the tuning of their chemical composition, for example, the doping on either M-, A- or X-site [3,4,5].

One of the recent goals is to obtain stable magnetic MAX-phases which can be also done via the chemical doping of the existing MAX-phases with magnetic elements [6,7]. The promising candidate for this purpose - $(Cr_{1-x}Mn_x)_2AlC$ MAX-phase. However, the successful doping of this compound, likewise the number of other MAX-phase family representatives, suffers from two main issues. One is the poor incorporation of the dopant atoms into the MAX-phase structure; another is the dramatic worsening of the samples phase purity, accompanying the increment of the dopant concentration, especially for bulk samples [8].

In this work two non-conventional techniques are described which can help one increase the doping level in quaternary MAX-phases, like $(Cr_{1-x}Mn_x)_2AlC$. One is the arc melting synthesis approach that is useful to obtain the samples with Mn concentrations up to 16 at.% which is half times more than it was achieved previously [8]. The increment of the doping level appears due to the influence of the high-energetic plasma arc, causing large temperatures up to 3000°C in the melt. This technique can be also optimized to overcome the second synthesis drawback and obtain highly phase-pure samples [9]. The second technique is the high-energy ball milling that can be applied for powder-form as-cast MAX-phases samples to further increase the doping level due to the additional incorporation of the excessing dopant in the miller.

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First-principles study: Spin-induced switching of the electronic states filling in Fe-based polyphthalocyanines

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Among the most promising candidates for 2D electronic devices are metal-incorporated polyphthalocyanines (MePPCs). Unique characteristics of the PPCs are caused by the organic matrix that can incorporate various transition metal atoms, forming an ordered structure with a period of around 1.1 nm (Fig. 1) [1]. The ability to choose the metal potentially allows a tunability of the material properties: MePPCs are expected to be ferromagnetic (Me=Mn), antiferromagnetic (Cr, Fe, Co, Cu) or diamagnetic (Ni, Zn) [2] materials, becoming a weak conductive half-metal materials. The first-principle study utilizing the QuantumATK [3] shows the large transformation of the electron states on the Fermi level for FePPC. The material has a direct (0.16 eV) and indirect (0.15 eV) insulating band gap for antiferromagnetic ordering of the Fe magnetic moments (Fig.1), while for any other ordering, the material has no band gap, becoming a conductive one. The result was found using spin-polarized GGA, where Heisenberg exchange interactions are included in consideration in relation to non-polarized GGA. Simulations were performed with varies initial spin configurations. The projected density of states (pDOS) also shows insulating behavior (Fig. 2). As a result, assuming possible temperature and external magnetic impact on Fe spin oscillations, these materials can work as ultrafast resistance oscillators or switchers, finding their application in terahertz electronics.

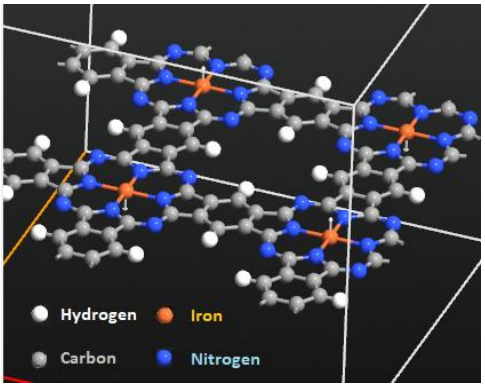

Fig. 1. Supercell of the FePPC with anti-ferromagnetic coupling of Fe atoms.

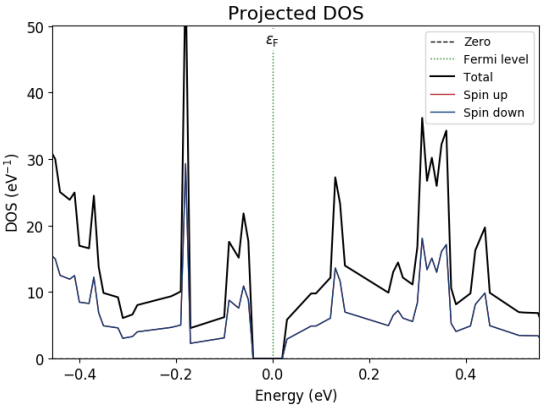

Fig. 2. Non-conductive gap on Fermi level of the pDOS for the antiferromagnetic configuration.

Acknowledgement

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Prediction of Al_2O_3 substrates' effect on magnetic properties of Mn_2GaC ultrathin films

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The process of epitaxial growth or deposition of high-quality thin films is almost always associated with a number of technological difficulties besides the choice of a surface for growth, preliminary screening of unpromising types of substrates becomes very important. In the case of magnetic thin films, for example Mn_2GaC, substrate-induced compression or expansion of the growing phase lattice provides an additional tool for controlling the magnetic properties of the film. A typical substrate for the synthesis of magnetic MAX phases is MgO(111) due to the low mismatch of the surface unit cell vectors with the vectors of the (0001) MAX phase plane. However, the resulting films of MAX phases are of low structural order. There are data on the growth of MAX phases on the Al_2O_3(0001) substrate [1]: although in this case the formation of MAX phases is accompanied by an increase in competitive phases, the quality of the crystal structure of the formed MAX phase is higher than on MgO(111). In this paper, we consider the question of growth possibility and the magnetic properties of the Mn_2GaC thin films on Al_2O_3 substrates of various orientations besides the Al_2O_3(0001).

The first stage of current work was to predict the most preferable interfaces between Mn_2GaC and Al_2O_3. Considering large number of atoms within the unit cells and, therefore, huge number of possible variants, we have chosen a pure geometric approach [2] for matching the atomic structures, which includes edge-to-edge lattice matching and near-coincidence site (NCS) density for generation and evaluation of possible orientational relationships and interfaces between the phases. Along with the experimentally observed $Mn_2GaC(0001)//Al_2O_3(0001)$ interface, the crystallogeometric approach predicts $Mn_2GaC(11\bar{2}1)//Al_2O_3(01\bar{1}1)$, $Mn_2GaC(01\bar{1}3)//Al_2O_3(11\bar{2}3)$, $Mn_2GaC(01\bar{1}2)//Al_2O_3(0001)$ and $Mn_2GaC(12\bar{3}6)//Al_2O_3(01\bar{1}2)$ as possible variants.

The second stage of current work used the lattice mismatches corresponding to the predicted variant to calculate the magnetic properties of strained Mn_2GaC thin film within the DFT-GGA method [3]. The results show significant effect of substrate-induced deformation on the energy of AFM→FM transition and spin polarization of the FM phase. The $Mn_2GaC(01\bar{1}3)$ thin films, which are expected to grow on $Al_2O_3(11\bar{2}3)$ surface, has energy difference between the AFM and FM phases of only 1.16 meV/Mn (compared to 2.63 in bulk) and this is equivalent to magnetic transition at fields of 10 Tesla only. The spin polarization of -28% (compared to -18% in bulk) is predicted for the FM phase of $Mn_2GaC(12\bar{3}6)//Al_2O_3(01\bar{1}2)$, which is only 1.54 meV/Mn higher than the AFM phase.

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Influence of the interaction of 2D Nb_2C and Nb_4C_3 MXenes with collagen and lysozyme on their colloidal and biological properties

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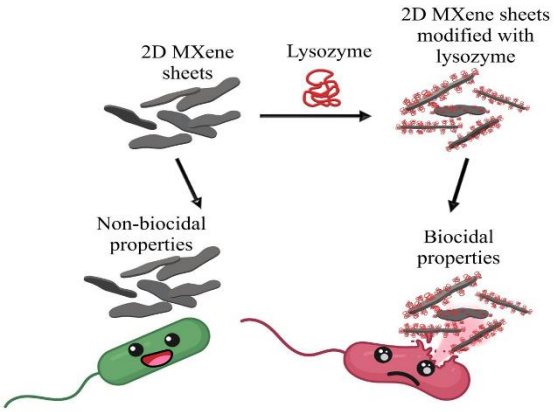
This work presents a comprehensive study on the surface-property changes of 2D flakes of MXenes (Nb_2C and Nb_4C_3) upon interacting with the cationic proteins – collagen and lysozyme, using time-resolved dynamic light scattering and zeta potential. The study aimed to investigate how MXenes stoichiometry, structure, surface chemistry, and exposure concentration affect its interactions with collagen and lysozyme. We found that the adsorption of the cationic proteins on 2D Nb_2C and Nb_4C_3 flakes occurred effectively, leading to changes in MXenes zeta potential in a concentration-dependent manner. The adsorption efficiency varied, depending on the surface chemistry and stoichiometry of the investigated MXenes. The zeta potential assays revealed that the adsorption mechanism for MXenes was mainly electrostatic.



We have shown that protein adsorption radically changes the physicochemical properties of MXen surfaces, which have a significant impact on their antibacterial and mycotoxic properties in relation to selected gram-positive bacteria *B. subtilis* and *S. aureus*, gram-negative *E. coli*, and *C. albicans* fungi.

Acknowledgements
The study was accomplished thanks to the funds allotted by the National Science Centre, Poland, within the framework of the research projects ‘PRELUDIUM 17’ no. UMO-2019/33/N/ST5/02095 and ‘SONATA BIS 7’ no. UMO-2017/26/E/ST8/01073

Poster reports

Ta/Au and Ta/Cu hybrid seed layers for gradual tailoring of texture and exchange bias in NiFe/IrMn exchange biased thin films

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Exchange bias in NiFe/IrMn bilayer has been tailored by modification of the ferromagnetic/antiferromagnetic (F/AF) interface texture through the thickness variations of Au and Cu layers in Ta/Au and Ta/Cu hybrid seed layer stacks. The revealed variations of exchange bias with Au and Cu seed layer thicknesses t_{Au} and t_{Cu} are gradual, but have opposite signs. For the Ta/Cu seed layer, the increase of t_{Cu} from 1 nm to 5 nm results in enhancement of exchange bias by 10 percent. For the Ta/Au seed layer, the similar variation of t_{Au} reduces the exchange bias by more than 30 percent. The effect correlates with the modifications of interface texture. The selection between Cu and Au in the seed layer stack defines this texture, as well as alignment of NiFe and IrMn crystallographic planes. The NiFe/IrMn films, grown on Ta(5 nm)/Cu (5 nm) seed layers, are of highly disordered multigrain structure, having wide angular distribution for orientations of crystallographic planes in respect to the interface plane. For the NiFe/IrMn thin films, grown on Ta (5 nm)/Au (5 nm) hybrid seed layer stack, both NiFe and IrMn layers have (111) texture with horizontally aligned (111) crystallographic planes.

Large enhancement of crystallinity for both NiFe and IrMn layers is revealed in the NiFe/IrMn films, grown on Ta/Au seed layer stacks. The use of Ta (5 nm)/Au (2 nm – 10 nm) stack instead of a single Ta (5 nm) seed layer results in amplification of XRD peak intensities for both NiFe and IrMn by more than 2 orders of magnitude. The XRD peak intensity for NiFe layer increases rapidly with Au layer thickness within 0 – 2 nm range and reaches a plateau, when the Au layer thickness is within 2 nm – 10 nm range. The TEM cross-section imaging of NiFe/IrMn thin film, grown on Ta (5 nm)/Au (5 nm) hybrid seed layer stack, reveals high crystallinity of both the NiFe and IrMn layers, with more than 25 subsequent horizontally aligned (111) planes, distinguishable in each layer. Using the Ta/Au seed layer stacks with the thicknesses of Au layer within 2 nm – 10 nm range, correspondent to the observed plateau of high crystallinity, facilitates the fabrication of NiFe/IrMn thin films with almost-epitaxial quality by using just a conventional DC magnetron sputtering technique.

Acknowledgement

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Transport properties of systematically disordered Cr2AlC films

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Nano-lamellar composite materials, known as MAX-phases, can possess a combination of ceramic and metallic properties. A prototype compound is Cr2AlC, formed from a unit cell of Cr2C sandwiched between atomic planes of Al, thereby imparting a good electrical conductivity, as well as mechanical stability, radiation and oxidation resistance [1, 2]. These properties rely on the lamellar structure of the compound, and systematic introduction of defects, such as displacing or doping atoms within the layers, has the potential to tune electron transport and modify magnetic properties [3]. An ideal tool for defect implantation is ionirradiation, available both in the form of a broad-beam for wafer-scale processing as well as focused ion-beams for device prototyping. Here we observe the modifications to the structural, transport and magnetic behavior of 500 nm thick Cr2AlC after irradiation with Co+ ions, and Ar+ noble gas ions as control. The films were irradiated with 450 keV of Co+ ions at fluences varying from 5×1012 to 5×1015 ions.cm-2, and the control samples with 400 keV Ar+ ions keeping the sample fluences. Structural analysis using XRD shows that ion-irradiation induces a suppression of the 0002 reflection, indicating a gradual decay of the nano-lamellar structure. Increasing ion-fluence also leads to an increase of the saturation magnetization at 1.5 K, whereby both Ar+ and Co+ cause an increased magnetization, respectively to 150 and 190 kA.m- 1, for the highest fluences used. Large variations of the transport properties are observed. Magnetoresistance (MR) in the non-irradiated sample shows a classical B2 dependency, even up to high temperatures. At Co+ fluences of 5×1013 ions.cm-2 the MR shows a two orders of magnitude increase, up to 3% (10 T) at 100 K. A similar effect also occurs for 5×1012 ions.cm- 2 Ar+ irradiated films, however with a smaller MR-increase. It appears that resistivity increases and the residual resistance ratio reduces with increasing fluence due to the introduction of disorder. These results show that ion irradiation induces significant changes in the transport properties of MAX phase materials, that will be further investigated. The systematic disordering of nano-laminated MAX phase films may therefore reveal interesting disorder and spin-related transport phenomena.

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Theoretical Prediction Structure of the M_2AX phase Fe_2AlC

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The layered MAX phases show remarkably hybrid metallic and ceramic characteristics. Like ceramics, they have low density, high strength, good corrosion and high temperature oxidation resistance; like metals, they are high electrical/thermal conductivities, relatively soft, appreciable machinability, thermal shock resistance and good damage and radiation tolerance. They are highly promising candidates for various applications, such as structural materials, corrosion protection, and nuclear fuel cladding coating materials [1].

Calculated the Fe_2AlC (figure 1) with space group $P6_3/mmc$ using B3LYP with DZVP basis set for optimization by CRYSTAL program. Cell parameters were obtained as a = 2.803 Å, c = 12.481 Å, the atom's spins for Fe = 1,82 which corresponds to Fe^{+2}, this suggests that this M_2AX phase exhibits magnetic properties and can be used in spintronics.

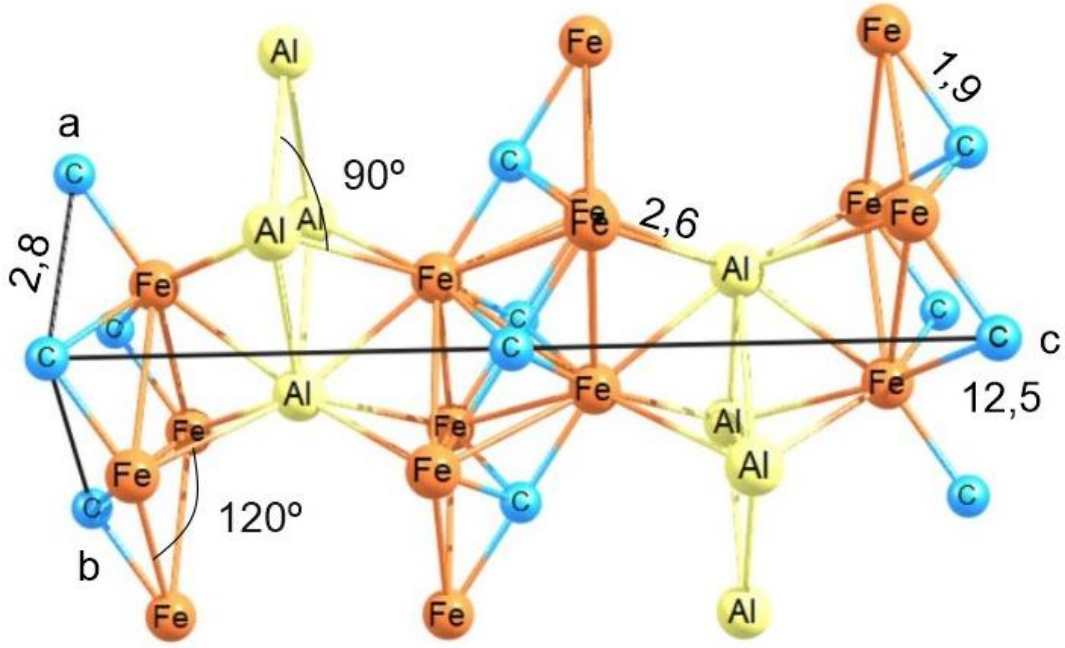

Figure 1. Structure of Fe_2AlC phase calculated by B3LYP/DZVP

Acknowledgement

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Atomic and electronic structure of MAX-phase Cr_2AlC studied by DFT calculations

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MAX – class of materials that was made syntactical, this class have a unic layered crystal lattice structure and some properties such as thermal and electricity conductivity, strength, corrosion, thermal and chemical resistance, and easy to mechanical treated[1].

In this work was found atomic and electronic structure of MAX-phase based on chromium, aluminum and carbon (Cr_2AlC) (figure 1), with using hybrid B3LYP functional by CRYSTAL program. Geometry was obtained with group symmetry $P6_3/mmc$. Total spin per cell 3.77 e^-, on the chromium atom S_{Cr}=1.19. It means that Cr exhibits an oxidation state +3. Charges were distributed as follows: on the chromium atom +0.53 e^-, on the aluminum -0.42 e^-, on the carbon -0.63 e^-. Calculations show good perspective for Cr_2AlC MAX-phase in magnetic applications.

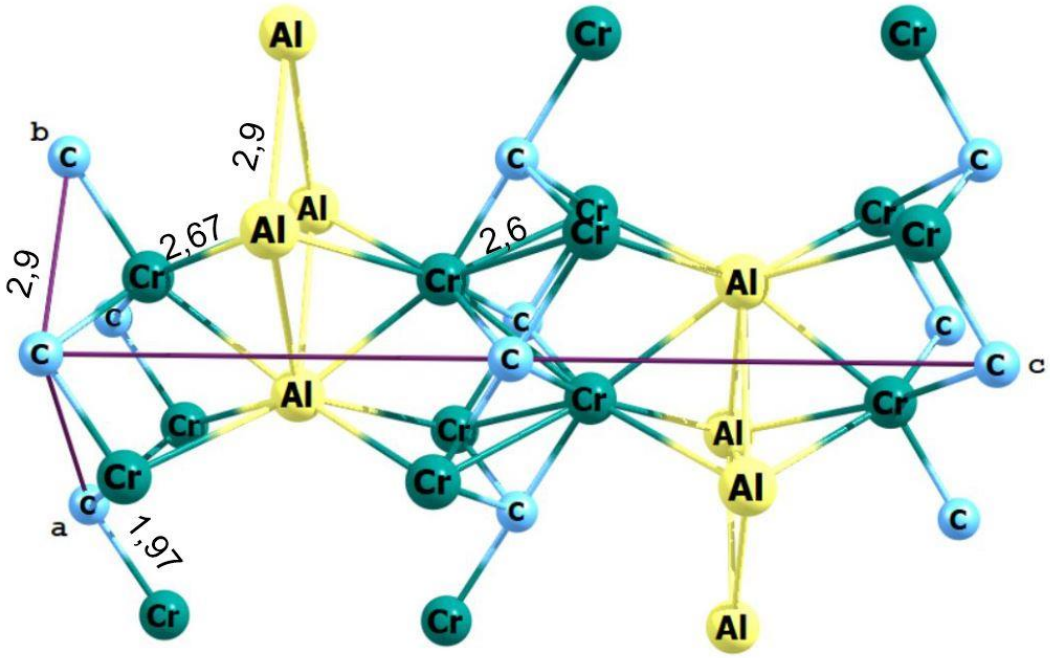

Figure 1. Structure of MAX-phase Cr_2AlC with space group $P6_3/mmc$, cell parameters a=2.9Å, b=2.9Å, c=12.46Å. a, b, c - lattice vectors.

Acknowledgement

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Structural and electronic properties of the MAX-phase Mn_2AlC finding by the hybrid functional B3LYP

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The MAX phases are a unique material with the properties of metals and ceramics. These phases are also called nano-laminates because of their layered structures, which consist of hexagonal carbide blocks $[M_{n+1}X_n]$ and planar A atomic sheets with a characteristic "zigzag" stacking along z axis in the sequence .../$[M_{n+1}X_n]$/A/$[M_{n+1}X_n]$/A/...The properties of MAX phases include high electrical and thermal conductivity, heat resistance, damage resistance, readily machinable, high modulus and low density [1].

The atomic and electronic structure of Mn_2AlC was found using hybrid B3LYP functional with DZVP basis set implemented by CRYSTAL [2]. The geometry (figure 1) was obtained in $P6_3/mmc$ symmetry. The total spin per cell was 11.23 e^-, while on the manganese atom S_{Mn} = 3.32 The charges were distributed as follows: on the manganese atom +0.28 e^-; aluminum -0.44 e^-; carbon -0.12 e^-. Calculations show that the intra-atomic bond for Mn_2AlC is of a mixed type. For example: inside blocks $[Mn_2C]$ there are covalent-ionic bonds Mn–C; metallic-like bonds Mn–Mn; between the blocks $[Mn_2C]$ and Al atomic sheets there are ionic bonds together with relatively weak covalent Mn–Al bonds.

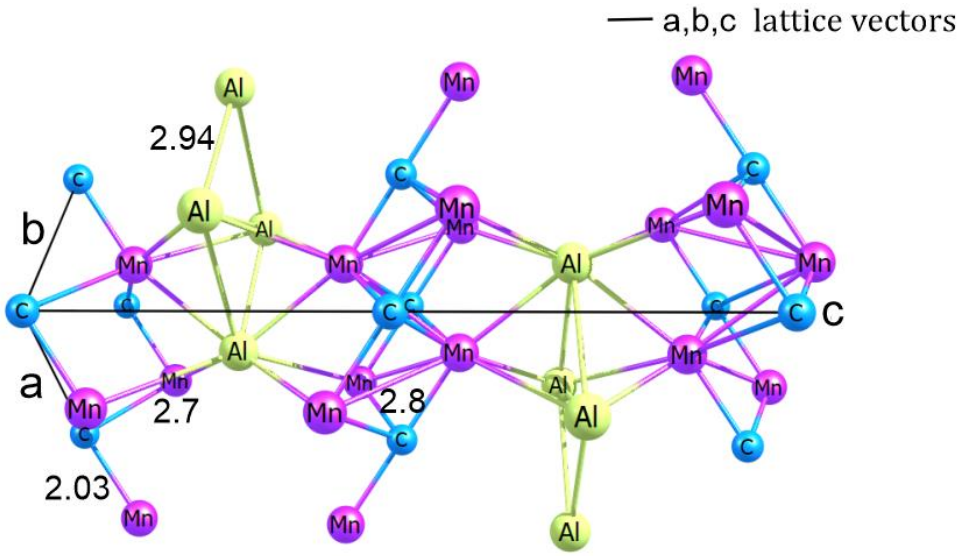

Figure 1. Atomic structure of Mn_2AlC. The cell parameters: a = 2.94 Å; b =2.94 Å; c=12.87 Å

Acknowledgement

This study was supported by the Government of the Russian Federation, the Mega-grant for the Creation of Competitive World-Class Laboratories, agreement no. 075-15-2019-1886.

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Thin films from Mn_3O_4 nanosheets. Preparation and morphological properties.

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Transition metal carbides and nitrides (MXenes), a family of two-dimensional (2D) inorganic compounds, are materials composed of multiple atomic layers of transition metal carbides, nitrides, or carbonitrides [1]. MXene is hydrophilic in nature, has excellent electronic conductivity and is easy to synthesize in large quantities in water [2, 3]. This unique combination of properties and ease of processing has allowed these materials to be used for a wide variety of applications, from energy storage to electromagnetic shielding, transparent conductive electrodes, electrocatalysis and many others. Composites MXene with Mn_3O_4 nanoparticles are being actively studied for effective use as catalysts in the design of energy storage devices [4, 5].

The study of the structural and morphological characteristics of MXene based on manganese is necessary for a deeper understanding of their properties and possibilities of application. Experimental work was carried out with samples of two-dimensional material based on manganese with the replacement of carbon atoms by oxygen atoms. Samples were obtained by chemical method. Sample A is Mn_3O_4 powder. Sample B is Mn_3O_4 functionalized with tetramethyl ammonium hydroxide (TMAOH).

Thin films of nanosheets Mn_3O_4 on the surface of silicon dioxide (SiO_2) were obtained using the apparatus for applying the solutions by centrifugation, using drop casting method. The thin films were made in two stages. 1. Dispersion of a sample of Mn_3O_4 powder in ethanol until a stable suspension is formed. 2. Application of the resulting suspension dropwise onto a rotating substrate. The drop casting method promotes uniform distribution of the dispersed solution over the substrate surface, rapid ethanol evaporation, and assembly of Mn_3O_4 particles. After the formation of thin films of Mn_3O_4, the morphological characteristics were studied. The microstructure of the images was studied using electron microscopy. Local elemental mapping of the surface was performed using energy dispersive X-ray spectroscopy. The characteristics of the obtained thin films from Mn_3O_4 nanosheets were studied using atomic force microscopy.

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Surface functionalization of 2D Mo2B2 MBenes: A First principle Approach

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The two-dimensional (2D) materials have received increasing attention due to their wide variety of applications in different fields. The 2D materials, such as the layers of transition metal borides called MBenes, are comparatively new [1, 2]. Similarly, like MXenes materials, which have been widely studied so far [3], MBenes can be chemically exfoliated from their bulk counterparts (MAB phases).

In this communication, we present a comprehensive ab initio studies of structural and electronic properties of 2D Mo2B2 structure, which is a representative system of 2D Mbene. The calculations were carried out within the framework of the Density Functional Theory (DFT) implemented in VASP software. We examine the orthorhombic and hexagonal Mo2B2 structures with various surface functionalization groups such as -F, -Cl, =O at different locations. The studies reveal, that in the case of the hexagonal crystal, the functional groups prefer to be adsorbed above the Boron atom in asymmetric configuration on two sides of Mo2B2 layer. Moreover, in the case of orthorhombic crystals, one of the functional groups is located exactly below to the Mo atom while the other one is located exactly above the boron atom at the bridge position between two Mo atoms. Furthermore, the adsorption and cohesive energies corroborate the stability of the functionalized structures. In addition, both functionalized and pristine structures exhibit metallic behavior.

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MXenes surface modification to obtain solid acids

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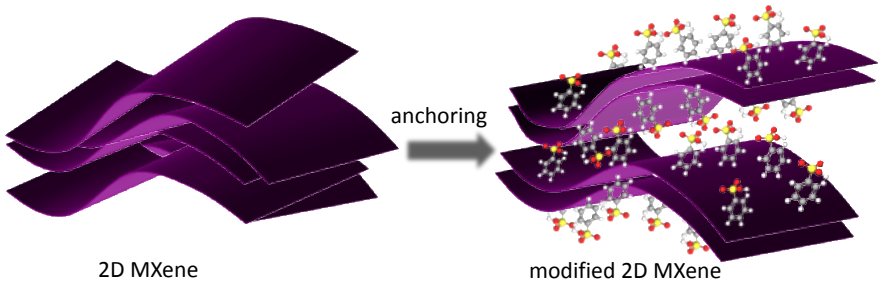
MXene, a novel family of two- dimensional (2D) metal carbides, with graphene-like structures is produced by etching of A from of MAX phases.[1] The *MXene* materials are described by a general formula of $M_{n+1}X_nT$, where M represents a transitional metal (TM), X is C and/or N and T is the surface termination (–O, –OH or –F groups), while the suffix "ene" emphasizes their resemblance to graphene.[2] A potentially useful approach to control *MXenes*' catalytic activity is *to manipulate their surface* chemistry. The surface terminations of *MXene* emerged during synthesis, have been foreseen to control different properties of the material, such as conductivity/superconductivity, band alignment, magnetism and even catalytic properties[3]. Although encouraging, these predictions lack direct experimental confirmation. Recently,[4] a combined experimental-theoretical report demonstrates that conductivity, can be controlled by adjusting the number and the types of termination (–OH, –F, =O).

Any solid acid is an alternative to the traditional liquid acids as recyclable and environmentally-safe acid catalysts. Acid solid materials show comparable results with that of acids in esterification of higher fatty acids.

Bearing this in mind and the fact that a solution to extend the *MXene*' acidity will be to control the number of –F terminations on the surface in the proximity of an acidic moiety (such as $–SO_3H$, or other acidic functional groups), this study proposes the synthesis of a MXene modified surface with an increased number of acidic terminations (Scheme 1).



By anchoring different aryl moieties to the surfaces containing acid functionalities, we have obtained materials with different acid density and strengths. Parameters such as concentration of the solution, temperature and grafting time was investigated.

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The Effect of Iron Substitution on the Structure and Electronic Properties of Cr_2SiC by theoretical method

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The search for new combinations of the MAX phase is still going on. Now the various characteristics of MAX phases such as Cr_2SiC and Fe_2SiC have been studied using density functional theory [1-3], however, the effect of iron substitution on the structure and electronic properties of Cr_2SiC has not been considered. The study of sequential substitution with one, two, and three iron atoms respectively are must be interesting.

The atomic and electronic structure of the MAX phase of $Cr_{2-x}Fe_xSiC$ was determined using the hybrid B3LYP functional and the CRYSTAL software package [4]. The results showed that the introduction of iron into the initial structure of the MAX phase of Cr_2SiC leads to an increase in the volume of the unit cell and is accompanied by a variation in the values of parameters *a* and *c*. There is a general increase in the spin and atomic charge of metals when iron is introduced into the structure. The considered compounds exhibit metallic conductivity. The studied properties of the quaternary MAX phase, substituted by iron, have not been previously calculated. Based on this, the results obtained can be considered as the first quantitative theoretical prediction.

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The flux-flow resistivity and Hall effect in highly layered electron-doped superconductor $Nd_{2-x}Ce_xCuO_{4+\delta}$

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The interaction and mutual influence of the charge and vortex systems in the mixed state of high-temperature superconductors (HTSC) is an important factor for understanding the physical processes and the practical application of these compounds.

The experimental results and analysis of the charge carriers transport and the vortices motion in highly layered electron-doped superconductor $Nd_{2-x}Ce_xCuO_4$ with x = 0.135, 0.145, 0.15 along CuO_2 conductive planes and between them with the changing of the external magnetic field will be presented.

The pulsed laser deposition technique was used to synthesize three types epitaxial monocrystalline films $Nd_{2-x}Ce_xCuO_4/SrTiO_3$:

- the *c*-axis of the $Nd_{2-x}Ce_xCuO_4$ lattice is perpendicular to the $SrTiO_3$ substrate plane;
- the *c*-axis is located in the plane of the substrate and is directed along the long side of the substrate;
- the *c*-axis is located in the plane of the substrate and is directed along the short side of the substrate.

It was found that in the presence of strong two-dimensional (2D) transport (incoherent tunneling and thermal activation of carriers through barriers between conducting planes), there is a thermally activated motion of vortices in a direction transverse to CuO_2 planes (lateral flow). The features of the behavior of the Hall resistivity between the CuO_2 planes indicate the motion of a system of Josephson vortices aligned in a magnetic field parallel to the CuO_2 planes, in a direction perpendicular to these planes, while overcoming their intrinsic pinning.

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Interface-induced Superconductivity by Quantum Mechanics

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Today, high temperature superconductivity (HTS) by the interface induced superconductivity mechanism [1] has been of great interest. However, the interface mechanism is not well understood and is better described by the historical exciton mechanism [2] of superconductivity based on attractive interaction between electrons even at high transition temperatures because of the excitation of excitons (hole-electron) pairs rather than phonons.

A decade ago, superconductivity [3] in thin nanoscale FM layers at ambient temperature was suggested based on excitons (hole-electron) pairs [2] produced in the film by Joule heating from read/write switching currents. Magnetic fields are not necessary. The simple QED theory of nanoscale heat transfer based on the Planck law which requires the heat capacity of the atom at the nanoscale to vanish was invoked which requires the conservation of Joule heat by the creation of EM waves across the film thickness as would occur in interface induced superconductivity. But at the nanoscale, the EM waves are beyond the UV in the EUV which ionizes the FM to produce the exciton (hole-electron) pairs that significantly lower the GMR to approach superconductivity. Paper [3] was recently updated [4] by modifying simple QED for the confinement of EM wave across the film.

In the presentation, the updated version [4] is followed and although based on spin current data from a decade ago shows simple QED based on the Planck law does not require phonons or magnetic fields to approach HTS. In this way, the Planck law of quantum mechanics by denying the atom heat capacity at the nanoscale requires the creation of non-thermal EM waves across the film thickness, the EM waves at EUV levels ionizing the film, thereby supporting the historic exciton (hole-electron) mechanism of superconductivity proposed here for interface induced superconductivity.

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UHV system for producing and studying of MAX phases by in situ spectral magneto-optical ellipsometry in a wide temperature range

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In recent years, researchers have been trying to create various new nanostructures with the required properties using various technologies. Layered structures "ferromagnetic metal/semiconductor", where Fe, Co, Ni, Mn can be used as metal, and Si, Ge can be used as semiconductor layers, are a good example of new materials. MAX phases are also of great interest npwadays due to unusual combinations of chemical, physical, electrical and mechanical properties, a special layered structure and a unique combination of the most demanded properties of metal and ceramics[1].

In these structures, it is important to pay attention to the formation, composition and properties of interlayer interfaces. However, not only the properties of the final structure are of interest, but also diagnosing materials in the process of their creation, which would make it possible to obtain structures with the desired characteristics, to synthesize nanomaterials with composition, structure, and properties controlled at the atomic and subatomic levels. The reflective spectral ellipsometry, being a non-destructive *in situ* method of surface analysis, is well suited for diagnostics [2,3,4]. This polarization optical technique allows one to obtain quantitative information about the structure and morphology of the surface of the sample under study, to find out its spectral optical and magneto-optical parameters directly during the formation of the structure, and to perform magneto-optical analysis of thin films when placing a ferromagnetic sample into an external magnetic field.

We describe an ultrahigh-vacuum setup in which the joint use of ellipsometric measuring equipment and methods for setting the temperature of the sample with the application of an external magnetic field of a given value to it was implemented [5,6]. The "ferromagnet/dielectric/semiconductor" structure was used to demonstrate the possibilities of the created ultrahigh-vacuum complex, i.e. to synthesize ferromagnetic nanostructures on the substrate surface with *in situ* non-destructive ellipsometric control and to carry out *in situ* studies of the obtained nanostructure by magneto-ellipsometry in the temperature range 85–1005 K in a single technological cycle.

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Enhanced Thermoelectric Properties of Double Transition Metal MXenes

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Thermoelectric (TE) materials are the promising candidate for renewable energy harvesting technology since it can generate electricity by recovering energy from the waste heat of environmental sources utilizing Seebeck effect.[1] The efficiency of TE device depends on transport properties (of both charge carrier plus lattice) of the material and is estimated by a dimensionless quantity called figure of merit (ZT). The best TE materials available today operating near room temperature, are doped semiconductor alloys of antimony and bismuth telluride having ZT of about 1, although for practical purposes, ZT value of 3-4 is desired.[2] In recent year, significant improvement on the performance of TE devices has been achieved in nanostructured TE materials, like layered 2D materials such as, MXene, family of transition-metal (TM) carbides, nitrides and carbonitrides.[1] Jing et al. predicted that figure of merit of p-type double TM MXene $Cr_2TiC_2(OH)_2$ could reach to 3.0 at 600K.[3]

Motivated by the above, in the present study [4] we focus on Mo and Ti based ordered double TM MXenes, namely $Ti_{3-x}Mo_xC_2T_2$ (x = 0.5, 1, 1.5, 2, 2.5) with surface termination T = -O/-F/-OH that can exist in two ordered phases, o-MXene and i-MXene. Employing first-principles calculations, we analyze their thermodynamic stability with respect to 1) ordered phases by computing formation energy and bond energy and 2) competting binary phases by ternary convex hull formation. Investigation of electronic and magnetic properties results in three semiconducting MXene stable in o-phase, namely $TiMo_2C_2F_2$, $TiMo_2C_2(OH)_2$ and $Ti_2MoC_2F_2$ having narrow band-gap with antiferromagnetic ground state, while rest are found to be metallic. In order to validate our scheme of transport calculation, we first determine the electrical transport properties of passivated n-type $TiMo_2C_2$ for which experimental results are available [5] and show good agreement with experimental data for the choice of passivation with O and OH. Our calculations show superior electrical transport properties of Ti_2MoC_2 compared to $TiMo_2C_2$ with a power factor of 10^4 $\mu W\ cm^{-1}\ K^{-2}$ at 300 K for a p-type carrier density of 10^{19} cm^{-3}. This leads to an exceptional ZT of 1.5 at 300 K and 3.1 at 800 K, the latter with a 27% efficiency thereby reaching close to the desired target. Our exercise should motivate experimental study of yet-to-be synthesized double TM MXene compound, Ti_2MoC_2.

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Choice of the DFT functional for calculation electronic properties of (CrFe)SiC MAX phases

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A wide family of structures is related to MAX phases and is of considerable interest to researchers. Main part of research involves calculating by *ab initio* methods. Obviously, the obtained results depend on the functional used in the calculation, the choice of which can be carried out from a wide range of options. Among the widely known and traditionally used functionals for the DFT method, such as GGA (PBE), hybrid (PBE0-13, B3LYP), meta-GGA (M06L, M06, M062X, M06HF) and range separated (CAM-B3LYP) DFT functional.

(CrFe)SiC refers to the MAX phase type 211. It can be considered as a Cr_2SiC crystalline phase in which some of Cr atoms are replaced by Fe. Moreover, if Cr_2SiC and Fe_2SiC have already been studied earlier [1–4], then (CrFe)SiC is studied for the first time. DFT calculations were performed using the Crystal package [5]. The analysis of the change in the of the optimized geometry parameters (CrFe)SiC in crystal cell and the atomic spins and charges of Fe and Cr were carry out depending on the used functional.

According to calculations the PBE0-13, B3LYP, M06 and CAM-B3LYP functionals give a satisfactory result and in good agreement with the literature data [1-3]. The PBE and M06L functionals lead to underestimation of the cell volume and on Fe and Cr charge, while M062X and M06HF overestimate the on Fe and Cr charge.

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Investigation of various spin configurations for the Co/Cu/Co system within the framework of ab initio calculations.

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Recently, the study of the properties of thin magnetic films has attracted great interest among researchers. Magnetic thin films are used as the base material for magnetic recording devices. Due to the rapid progress taking place in the magnetic recording industry, the calculation of magnetic characteristics in Co films separated by non-magnetic layers has become an important issue in the field of solid state physics.

In this work, we performed numerical studies of the energy and magnetic properties of the Co / Cu / Co system within the framework of the spin density functional method.

The total energy of the system was calculated depending on the convergence parameters: the size of the Monkhorst-Pack grid in the reciprocal lattice (Kpoints) and the cutoff energy (Encut). Beginning with the cutoff energy Encut = 500 eV, the total energy of the supercell changes insignificantly (± 0.001 eV). We have chosen the optimal value Encut = 600 eV. The convergence of the total supercell energy (with an accuracy of ± 0.001 eV) in terms of the number of Kpoints is observed at Kpoints = 20-28, while for the difference between the energies of the AFM and FM configurations, convergence is observed only starting from Kpoints> 36. The optimal value was chosen Kpoints = 48.

Calculations of the energy difference between AFM and FM spin configurations depending on the number of substrate layers from 3 to 9 monolayers and magnetic material from 1 to 3 monolayers showed that the most energetically favorable ferromagnetic configuration becomes when the number of substrate layers is 9 monolayers and the magnetic material in 3 monolayers with $\Delta E = 22$ meV. In other cases, it fluctuates around zero, which does not allow making an unambiguous conclusion.

The study of the dependence of the magnetic properties of the system on the number of Co monolayers showed that the values of the magnetic moment obtained in the course of calculations are in good agreement with the experimental data of other researchers. Thus, the value of the magnetic moment for a cobalt monolayer on the surface of the (100) face is $\mu = 1.826$ (1) μB.

Calculations of the energy of magnetic anisotropy depending on the orientation of the surface face showed that for the faces (100) and (111) the most energetically favorable direction of the magnetic moments is parallel to the plane of the film. A weak perpendicular magnetic anisotropy is obtained for the (110) face.

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Structural and electronic properties of the heterostructures based on Me_2AlC-phase predicted by quantum chemistry calculations

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The MAX phases are interesting material with the unique properties for wide application in technology. The atomic and electronic structure of Me_2AlC (Me = Fe, Cr, Mn) was found using hybrid B3LYP functional with DZVP basis set by CRYSTAL program [1]. The geometry was obtained in high symmetry ($P6_3/mmc$). To simulate the possible magnetic properties, structures with different spins were calculated. All MAX phases showed high spin on metal atoms. Then, carbon-terminated slab structures were obtained from these structures. Then various materials were placed on these slabs, such as graphene, *h*-BN, *g*-C_3N_4. These structures showed high stability, which shows the prospect of using such heterostructures in various applications in electronics.

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