Warsaw, 13.10.2023

Attachment no. 3

Summary of Professional Accomplishments

(english)

Dr. Magdalena Popielska (Birowska)

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CHAPTER 1

Personal data

Name: Magdalena Popielska (family name *Birowska*)
I publish under my family name.
Date and place of birth: 02.03.1984, Cieszyn (Poland)
married, two children
personal website: https://www.fuw.edu.pl/ birowska/

CHAPTER 2

Diplomas, degrees conferred in specific areas

November 2014 - Ph.D. degree
Institute of Theoretical Physics, Faculty of Physics, University of Warsaw (UW). Doctoral dissertation entitled: *"Uniaxial Magnetic Anisotropy in Diluted Magnetic Semiconductor (Ga,Mn)As"*; under the supervision of Prof. Dr. h.c. Jacek A. Majewski;
discipline: physical sciences

December 2008 - MSc in Biophysics
Faculty of Physics, Jagiellonian University, Cracow. Dissertation entitled: *"Application of selected physical methods in studies of red blood cells"*; under the supervision of Dr. h.c. Kvetoslava Burda,
discipline: physical sciences.

June 2008 - MSc in Physics (with honours)
Faculty of Physics, Jagiellonian University, Cracow. Dissertation entitled: *"Application of LDA methods for calculation of electronic states in selected nanoscopic systems"*; under the supervision of Prof. Dr. h.c. Józef Spałek,
discipline: physical sciences.

CHAPTER 3

Information on employment in research institutes or faculties/departments

- Since X.2020r. - present - **Assistant Professor**, Institute of Theoretical Physics, Faculty of Physics, UW.
- VIII.2017r. - VIII.2021r. - **Adjunct**, Principal Investigator (PI) of research project (SONATA, NCN), Institute of Theoretical Physics, Faculty of Physics, UW. Project entitled: *Theoretical study of structural, electronic, magnetic, and optical properties of the van der Waals heterostructures containing 2D layered materials*. Employment extended in this project by half a year due to maternity leave.
- XII.2014r. - VII.2017r. **Post-doc**, Institute of Theoretical Physics, Faculty of Physics, UW. Postdoc in project HARMONIA V, National Science Center (NCN), entitled: *Modeling of graphene structures coupled to metal and insulators*. Employment extended in this project by half a year due to maternity leave.

CHAPTER 4

Description of the achievements

As a scientific achievements, in accordance with Article 219 (4) of the Act of 20 July 2018[1], I indicate a cycle of 8 thematically related publications with a common title:

Tunable physical properties of layered crystals examined by ab initio approach.

The cycle of thematically related publications were published in years of 2019-2023 [2, 4, 6–8, 32, 34, 40]):

[1] *Higher Education and Science Law, Art. 219 (2018), Chapter 3 pages 121-122*

H1. **M. Birowska**; J. Urban, M. Baranowski, D. Maude; P. Płochocka, N. Gonzalez Szwacki, *The impact of hexagonal boron nitride encapsulation on the structural and vibrational properties of few layer black phosphorus*, Nanotech. 30, 195201 (2019)
IF: **3.953**, MNiSW score: **100 pts.**

H2. T. Necio, **M. Birowska**; *Supercell-core software: a useful tool to generate an optimal supercell for vertically stacked nanomaterials*, AIP Advances 10, 105105 (2020)
IF: **1.697**, MNiSW score: **70 pts.**

H3. **M. Birowska**, M.E. Marchwiay, C. Draxl, J.A. Majewski; *Assessment of approaches for dispersive forces employing graphone as a case study*, Computational Materials Science 186, 109940 (2021)
IF: **3.572**, MNiSW score: **100 pts.**

H4. **M. Birowska**, Paulo E. Faria Junior, J. Fabian, J. Kunstmann; *Large exciton binding energies in $MnPS_3$ as a case study of a van der Waals layered magnet*, Physical Review B, 103, L121108 (2021)
IF: **3.908**, MNiSW score: **140 pts.**

H5. M. Rybak, T. Woźniak, **M. Birowska**, F. Dybała, A. Segura, K. J. Kapcia, P. Scharoch and R. Kudrawiec; *Stress-Tuned Optical Transitions in Layered 1T-MX_2 (M=Hf, Zr, Sn; X=S, Se) Crystals*, Nanomaterials 12, 3433 (2022)
IF: **5.719**, MNiSW score:**100 pts.**

H6. C. Autieri, G. Cuono, C. Noce, M. Rybak, K. M. Kotur, C. E. Agrapidis, K. Wohlfeld, **M. Birowska**; *Limited ferromagnetic interactions in monolayers of MPS_3 (M=Mn, Ni)*, Journal of Physical Chemistry C 126, 6791 (2022)
IF: **4.177**, MNiSW score: **140 pts.**

H7. R. Basnet, K. Kotur, M. Rybak, C. Stephenson, S. Bishop, C. Autieri, **M. Birowska**, J. Hu, ; *Controlling magnetic exchange and anisotropy by non-magnetic ligand substitution in layered MPX_3 (M = Ni, Mn; X = S, Se)*, Phys. Rev. Research 4, 023256 (2022)
IF: **4.2**, MNiSW score: **40 pts.**

H8. W.M. Linhart, M. Rybak, **M. Birowska**, P. Scharoch, K. Mosina, V. Mazanek, D. Kaczorowski, Z. Sofer, R. Kudrawiec; *Optical markers of magnetic phase transition in CrSBr*, Journal of Materials Chemistry C 11, 8423-8430 (2023)
IF: **8.067**, MNiSW score: **140 pts.**

Description of the habilitation thesis

"Tunable physical properties of layered crystals examined by ab initio approach"

1. Introduction

"There is plenty of room at the bottom" is one of the famous quotes by physicist Richard Feynman, who said this sentence while delivering a lecture at a meeting of the American Physical Society on December 29, 1959 [15]. He discussed the possibilities of manipulating matter at the atomic scale, essentially exploring the world of nanotechnology before the term was even invented. At that time, he realized that many exciting scientific phenomena in layered materials would be revealed if we were able to control the number of layers in layered materials.

In particular, the successful isolation of graphene boosted up the research on nanomaterials, when it was realized that the 2D materials are accessible experimentally using a simple scotch tape technique [37]. In particular, electrons in graphene can be described as massless Dirac fermions exhibiting extremely high carrier mobility, even at room temperature [3]. However, graphene is a semi-metallic material, which limits its applications in transistor devices [42]. The ability to switch electrical signals is at the heart of all modern electronic devices, from computers to smartphones. Although, many approaches have been applied to open the band gap of graphene [14], the solid state community search for other 2D strutures derived from layered materials exhibiting the semiconducting properties. Nowadays, a rich variety of layered materials are accessible including insulators, metals, ferroelectrics, superconductors, and magnetic etc. However, reducing the dimensions from 3D to 2D does not guarantee that the properties manifested in 3D forms will be persistent down to monolayer limit. On the other hand, layered materials offer a great opportunity to access new dimensionality-dependent phenomena. In particular, the vdW layered materials benefits over conventional bulk materials with covalent bonds, namely, they can be largely decouple from the substrates due to weak dispersive forces between the adjacent layers. Moreover, they are mechanically flexible and readily amenable to chemical functionalization. This makes them accessible, easy to engineer and easy to integrate into various heterostructures [36]. The tunable properties of layered materials make them highly versatile for a wide range of applications, from electronics and photonics to energy conversion and sensing.

There are many factors that can be applied to tune the physical properties of layered materials including their thickness, layer stacking, chemical functionalisation, intercollation, strain-engineering, doping or external stimuli such as electric field. Since last 4 years, my scientific research have been particularly related to the topic of layered materials, where several aspects in the context of the tunable properties have been considered:

(I) strain-induced physical effects;

(II) substrate-induced effects;

(III) impact of quantum confinement;

(IV) doping effect at atomic limit;

(V) changes in physical properties induced by magnetic ordering of spins.

These aspects constitute the heart of my scientific achievements presented in this habilitation thesis. They are discussed further by examining various layered materials including:

- graphene;
- BP - black phosphorus;
- hBN - hexagonal boron nitride;
- TMDs - transition metal dichalcogenides (MX_2, M=Hf, Zr, Sn; X=S, Se);
- MPX_3 - transition metal trichalcogenides (M=Mn, Ni, X=S, Se);
- CrSBr.

To provide a reliable quantitative description of the aforementioned effects, most of the calculations have been performed within the framework of density functional theory (DFT). For particular properties such as excitonic features (versatile formalism of the Bethe-Salpeter equation) or magnetic phenomena (Hubbard models), the effective models parameterized by the *ab initio* calculations have been utilized.

2. Methodology

Ab initio calculations in the framework of the density functional theory (DFT) [23] are currently one of the most important computational tools to examine the atomistic properties of the nanomaterials. DFT is a crucial building block for modern theoretical physics, chemistry, and engineering. Currently, this approach is being considered as one of the most accurate methods of predicting the electronic structure of nanomaterials and it is still under extensive development. This computational methodology does not only provide physico-chemical explanations in interpreting experimental data, but also predicts and exploits properties that are difficult to measure with good accuracy. The key issue in DFT methodology is based on transferring the complexity of the electron-electron interaction to the effective single-particle equation determined by the approximate exchange-correlation (XC) functional. Generally, the accuracy of DFT method strongly depends on the choice of the XC functional [45]. Most of DFT calculations relies on the firstly developed local (spin) density approximations (LSDA) [26] or on the generalized gradient approximation (GGA) [38]. However, it is well known that these XC functionals just partially cancelled out a self-interaction of electron with its own charge density, resulting in severe underestimation of the bands gap (E_g) of semiconductors, as well as the spatial delocalisation of electrons from *d*- and *f*-shells. The consequence might be unwanted metallisation of the system or incorrectly predicted magnetic moments localized on these atoms. One of the possible improvements is a DFT+U approach (see Ref. [22] for review), in which a repulsion between electrons (usually from *d, f* orbitals) localized on a given atom is included (Hubbard U term).

The another approach that can be applied is hybrid functionals, where the combination of Hartree-Fock (HF) and DFT functionals are used (see Ref. [25] for review). In the HF theory, the exchange term cancels a self-interaction error occurring in the Hartree

part (Coulomb repulsion term). Note, that the electron correlation part is not included in HF theory. The exchange term exhibits a long-range nature and it is unscreened, which results in high excitation energies and a large overestimation of E_g in HF method. Hence, the combination of the underestimated band gap obtained using LDA (or GGA) and overestimated HF's band gap generally provides more realistic values of E_g, being advantage of using hybrid functionals. It is worth to mention that the self-interaction error is not fully eliminated in this approach.

In addition, vdW layered systems require the proper description of the dispersion forces, which originated from the electron correlations (electrostatic forces between induced-dipoles, also known as London or vdW forces). Note, that there is a lack of the long range van der Waals interaction in the standard XC functionals. These dispersive forces can be included at different levels of theory within Grimme's semiempirical force field corrections (DFT-D) [21], and regarding a non-local van der Waals density functionals (vdW-DF) (see Ref. [9] for review). In addition, for systems in which spin-orbit interaction is relevant the noncollinear formalism was included. All aforementioned functionalities and approaches are implemented in and VASP software [27, 28] and have been used in **[H1-H8]** publications. The calculations were executed using computational facilities installed at Interdisciplinary Center of Modeling ICM, UW and at Cyfronet in Cracow, within PL-Grid Polish Infrastructure for Supporting Computational Science in the European Research Space.

2.1. Strain-induced physical effects in layered materials (H2, H5).

The strain itself refers to a novel research field in solid state physics, called straintronics [10], where physical phenomena induced by strains, and strain engineering are exploited to develop new devices. The lattice mismatch at the interface of two conventional semiconducting materials such as Si, Ge, and III-V materials like InAs/GaAs is a critical issue, thus limiting the exploration of high-performance devices. It can induced stress at the interface leading to the formation of defects, such as cracks or dislocations, which can degrade the overall performance of the materials. Additionally, dangling bonds at the interface are created, hence leading to atomic intermixing, which might greatly modify the electronic properties. The vertically stacked layers provides new strain relaxation mechanisms at unusually high lattice mismatch, due to the weak van der Waals forces between the adjacent layers, enabling strain-induced band structure engineering. These materials represent a new class of hybrid crystals known as van der Waals (vdW) heterostructures [16], which properties can be superior compared to isolated 2D materials, and they can depend on the mutual arrangement of the adjacent layers. In particular, an unconventional superconductivity found in graphene can be precisely controlled by a "twist angle" of the adjacent atomic layers [11, 12].

The modeling of different types of 2D layers mostly relies on electronic band structure calculations in the framework of DFT, which is currently considered to be one of the most accurate *ab initio* methods. The commonly available quantum mechanical packages, such as VASP [27,28] Quantum Espresso [17] and SIESTA [47] exploit periodic boundary

conditions, where supercell approach is used. Such calculations are feasible by up to few hundreds of atoms. However, stacking adjacent layers with different lattice parameters or different lateral crystal symmetries usually require very large supercell, consisting thousands of atoms within it. In the paper **[H2]**, we present a developed software (open-source free software, available as a Python module [1]) based on commensurability condition, which implies long-range crystalline order in the sets of lattice planes that constituting the layered hybrid material. The software enables finding the optimal supercell, i.e., those with small size and low strain distribution. Particularly, our developed package searches through all possible superperiodicities originating from multiples of primary cells for a given rotation angle between the top and bottom 2D lattices. The software allows for determination of the optimal "magic angles" between the adjacent vertically stacked layers and the resulting moiré patterns. Software also enables construction of the optimal supercells based on the twist angle(s), and studying strained supercells in order to examine the influence of the strain distribution on the various properties of layered materials. Our software correctly predicts magic angles and moire patterns of previously reported graphene layers based on STM experiments. The strain distribution can be experimentally explored via variety of methods, such as atomic force microscopy (AFM), scanning tunneling microscopy (STM), and/or Raman spectroscopy [52, 53].

Strain engineering has been widely established in the semiconductor industry. Particularly, when the uniaxial or biaxial tensile strain is applied to the channel of a silicon transistor, the carrier mobility can be greatly enhanced [51]. In spite of that, conventional semiconductor bulk single crystals only sustained very small strains, that greatly limits the further application of strain modulation. Compared with bulk materials, 2D crystals have stronger deformation capacity and can sustain larger elastic strains without fracture, as reported previously for graphene layer that can withstand up to 25 % without fracture [13]. In the paper **[H5]** we have determined optically active transitions in bulk MX_2 compounds (M=Hf, Zr, Sn; X=S, Se) which crystalline in 1T polytype. These transitions have been analyzed under external hydrostatic, uniaxial, and biaxial stresses. Generally, the studied transitions are optically active, exhibiting in-plane polarization of light. We quantify their energy trends under various external stresses by determining the linear pressure coefficients. The largest pressure coefficients are predicted under uniaxial stresses for Sn containing structures. The negative pressure coefficients pointing to the narrowing of the band gap. The semiconducting-to-metal transition are predicted under hydrostatic pressure. Our calculated pressure coefficients are in excellent agreement with experimental values measured for the absorption edges of HfS_2 and $HfSe_2$. Our computational strategy based on their pressure evolution provides a new tool for identification of optical peaks for other layered materials.

2.2. Substrate-induced physical effects in layered materials (H1, H3, H4)

The role of the substrate in layered materials is crucial issue, as it can profoundly affect its properties due to proximity effects, structure, and performance. On the other hand, it provides mechanical support to the layered material, ensuring its stability and preventing deformation or damage. It is well know that many of the layered materials are

sensitive to the local environment and ambient conditions. The black phosphorus (BP) is an extreme case of sensitivity to moisture, which might lead to its degradation within in few minutes. One of the solution to prevent its structural and chemical degradation can be its encapsulation by other 2D material.

In the paper **[H1]**, we explore the impact of the hBN substrate on the structural and elastic properties of BP layers. We unveil, that the hBN encapsulation modifies the structural parameters of the constituent BP layers. In particular, the hBN encapsulation flattens the puckered structure of the BP layers via an the expansion of the intralayer bonds and pucker angle. Notably, structural changes are directly related to vibrational properties of BP. The strong interaction between the individual layers of BP results in the different stiffness of the surface and inner layers. This is directly reflected by the splitting of the high frequency optical Raman mode A_g^1. In general, hBN encapsulation imposes the strain formation in the BP layers, causing the additional redshift of the optically active Raman A_g^1 mode. The encapsulation strategy opens the door to substrate controlled strain engineering in atomically thin crystals.

The crucial role of a substrate has also been pointed out for the graphene hydrogenation process [35, 39, 54]. Our research **[H3]** shed light on the physical mechanisms of graphene hydrogenation both in vacuum and in the proximity of metallic surface. In particular, our results reveal that the adsorption of hydrogen atoms to the graphene layer is strongly affected by the Ni substrate, which is a consequence of the forming semi-covalent bonds between the graphene and Ni substrate. Additionally, the adsorption of hydrogen layer to graphene is stronger in the presence of the metallic surface. In this regard, the Ni surface acts as a stabilising substrate facilitating the formation of the graphone (semihydrogenated graphene).

The impact of substrate is a critical issue regarding the optoelectronic applications. In particular, the dielectric constant is a fundamental optical parameter that defines materials' ability to screen electric field, making it fundamental material property in determining the performance and functionality of devices based on 2D materials. In particular, the excitonic properties are strongly related to the dielectric screening of the environment. In the paper **[H4]**, we show that for monolayer of MPX_3, the exciton binding energy can be reduced by about two to three times in the case of SiO_2 and hBN substrates, respectively. The dielectric screening of the surroundings is a critical issue that significantly modifies the exciton properties of 2D materials.

2.3. Impact of quantum confinement on physical properties [H1, H4]

In bulk materials, electrons occupy energy bands with continuous energy levels. In contrast, by reducing the thickness of a layered material to only a few layers or even a single layer, the confinement in the out-of-plane direction becomes significant leading to quantized energy levels in reduced dimension. The layer-dependent properties in vdW materials are extensively explored since the first observation of the quantum size effect reported in 2010 [49]. The discovery of the direct band gap in single layer of MoS_2, which is an indirect band gap in the bulk form, sparked the excitement of 2D research community, providing opportunities for engineering the electronic structure of matter at the nanoscale

level.

In paper **[H4]** we have demonstrated that the band gap of $MnPS_3$ undergoes indirect to direct transitions, once the bulk is reduced to monolayer limit, accompanied by a small change in lattice parameters of up to 0.02 Å. The band extrema occurs at high symmetry point K and non-special k-points, for ML and bulk, respectively. Additionally, the bandgap increases up to 200 meV for monolayer compared to bulk material, depending on the computational approach. Regarding the curvature of the band extrema, which are quantified by effective mass tensor components, the calculations reveal comparable in-plane components for ML and bulk systems. The discrepancies are observed for the calculated principle reciprocal axes, which coincide with the Cartesian reciprocal axes for ML systems. In the case of the bulk system only one axis is parallel to [010] crystallographic direction, the other two are shifted from Cartesian reciprocal axes.

Remarkably, the quantum confinement effect is visible in 4-fold decrease of the exciton binding energy, which have been predicted for $MnPS_3$ material for first time in **[H4]**, within the versatile formalism of the Bethe-Salpeter equation (BSE) with effective models parameterized by DFT+U calculations. Particularly, the giant exciton binding energy is reported for ML equal to 1 eV in vacuum, which is reduced to 100-200 meV in bulk phase, greatly exceeding corresponding values for widely examine transition metal dichalcogenides (TMDs). Moreover, the layer dependent vibrational properties are observed for BP **[H1]**, where the large blueshift of the A_g^1 mode is reported for monolayer in respect to 5-layered system. Additionally, the BP layers, show anomalous evolution of phonon frequencies, as number of layers increases.

2.4. Doping effect in layered materials at atomic limit [H3, H6, H7]

Doping refers to the intentional introduction of certain types of impurities into a material in order to modify its properties. Doping is a crucial process in semiconductor fabrication, enabling the design and production of various electronic devices with specific electrical characteristics. Particularly, the ion-implementation in Si technologies have played an important role in establishing silicon complementary metal–oxide–semiconductor (CMOS) techniques as the paramount approach in the electronics industry. However, an ion-implementation technique is a challenge for the layered materials, as it can lead to damage to the atomically thin crystal structure. Hence, alternative approaches or new ones continue to emerged. The recent report has shown that for transistor built on vdW heterostructure, in which the MoS_2 layer can be remotely doped via controlled charge transfer from molecular dopants attached to its surface [31].

In paper **[H3]**, we have examined the energetics and structural changes induces by hydrogen attachments to the graphene surface. We have demonstrated that the adsorption energy profile exhibits two minima. The first one corresponds to strong adsorption - chemisorption, at the distance between the Hydrogen atom and graphene equal to 1.2 Å. The second one, is a weak adsorption of the van der Waals type (physisorption), occurring at the distance about 2.5-3 Å, depending on the type of exchange-correlation functional and the vdW method employed. The strong adsorption of the Hydrogen atoms results in large structural changes of graphene layer, namely its buckling by up to 0.33 Å. Such large

structural changes in graphene layer, may affect its electronic properties, as the band gap can be controlled by the hydrogenation pattern and can be tuned as wide as 3.9 eV by varying hydrogen coverage [48].

The doping strategy can be also experimentally realized in series of layered material via substitutional doping, as have been widely reported for layered MPX_3 materials [5,19,20,43,44]. In particular, in the paper **[H7]** we have examined the non-magnetic, chalcogen substitution in layered systems $MnPS_{3-x}Se_x$ and $NiPS_{3-x}Se_x$ ($0 \leq x \geq 3$). Our work reveals different trend of the Néel temperature under the change of the concentration of the dopants x in Mn and Ni contained materials, with stronger composition dependence in $NiPS_{3-x}Se_x$. This phenomena is attributed to the larger magnitudes of exchange couplings for Ni structures in comparison to corresponding Mn counterparts. We have demonstrated that the dominant exchange interaction, namely direct M-M interaction in $MnPS_3$, whereas superexchange M-X-M interaction is relevant for the first nearest neighbours (NN) in $NiPS_3$ [2]. Additionally, we have shown that chalcogen substitution effectively controls the magnetic anisotropy, which is reflected by the efficient tuning of the magnetic easy axis and spin flop (SF) transition. Such tunable magnetism revealed by non-magnetic substitutions provides a useful method to engineer low-dimensional magnetism and gives further insights for the development of magnetic materials-based nanodevices.

The magnetic doping realized in MPX_3 crystals is systematically considered in the paper **[H6]**. In this work, we examine theoretically various substantial magnetic doping considering mixed spins and mixed nearest-neighbor magnetic interactions of the alloys $(M_{3/4},X_{1/4})PS_3$ for M=Mn, Ni, and X=Mn, Ni, Cr. We systematically explore the mixed exchange coupling parameters between the metal host and dopant atom within DFT + U approach, assuming certain concentration of dopants. We have demonstrated, that magnetic impurities do not affect the magnetic ordering observed in the pure phases. However, unlike for the hosts, the first and second (dopant–host) exchange couplings are of similar order of magnitude. This might lead to the frustration in the case of antiferromagnetic coupling and may be one of the reasons of the observed lower magnetic ordering temperature of the alloying systems. Additionally, we have shown that the Mn and Ni dopants have tendency to cluster, while the Cr ions prefer to be randomly distributed over the host. All considered alloys are Mott insulating, although with generally smaller band gaps than those of the corresponding hosts. Additionally, ferromagnetism may not be easily induced by such a kind of elemental doping, hence, the MPX_3 layered materials can be regarded as robust AFM crystals. Nevertheless, for certain arrangement of the dopants in the $NiPS_3$ host, the ferrimagnetic state appears, as the dopants have different spins than the pure phases.

2.5. Changes in physical properties induced by magnetic ordering of spins in layered crystals [H4, H8]

The family of two-dimensional (2D) materials covers almost all properties, including systems exhibiting insulating, metallic, superconducting and nowadays also magnetic behavior. Although, many efforts has been put to induce the magnetism in thin films, the truly 2D magnets had been missing until 2017, when intrinsic magnetism in $Cr_2Ge_2Te_6$ [24] and CrI_3 [18] atomically thin layers revealed by scanning magneto-optic

Kerr microscopy. Until recently it was believed that, the magnetic order could not survive in 2D limit, due to the enhanced thermal fluctuation revealed by Mermin-Wagner theorem [33]. However, the recent reports have demonstrated that magnetic anisotropy could stabilize magnetic order by opening up an excitation gap, and thus, suppressing the effect of the thermal fluctuations [30]. In addition, the theoretical results, based on the *ab initio* calculations also reported stable magnetic monolayers [41, 46], as well as there had been some experimental reports in late 2016, of few layer of $NiPS_3$ that exhibit magnetic order revealed by Raman spectroscopy [29].

Additionally, one of the representatives of magnetic layered materials is the family of transition metal trichalcogenides MPX_3, where M=V, Cr, Mn, Fe, Ni, Cu, Zn, X=S, Se, Te [46]. These materials exhibit intrinsic in-plane antiferromagnetic orderings (AFM, zero net magnetization), providing ideal platform for studying the intrinsic intralayer magnetism. Note, that AFM materials are commonly found in nature and they are permitted in each magnetic symmetry group, albeit they are less utilized than ferromagnets (FMs). The great challenge in respect to 2D AFM crystals, is how the AFM ordering can be manipulated and read by conventional magnetic techniques. Specifically, the magnetic measurements such as SQUID or neutron scattering methods, are insufficient technique to investigate 2D magnets, due to the size of the sample. However, the optical measurements such as Raman Spectroscopy and second harmonic generation (SHG) [50], demonstrate the indirect strategy to probe the magnetism in vdW layered magnets. On the other hand theoretical *ab initio* calculations can infer physical properties that are sensitive to magnetic ordering.

In the paper **[H4]** we demonstrate that the magnetic ordering strongly affects electronic, transport and optical properties. In general, our results reveal a robust sensitivity of AFM arrangement of spins on the electronic features such as band alignments, band crossing and band gaps. In particular, we show that the electronic band gap relies on the magnetic state of the Mn atoms, differ from few tens to few hundredths of eV from each other, irrespective to Hubbard U parameter. The smallest band gap is revealed for AFM-stripy spin configuration (1.8 eV for DFT+U=3eV), while it is 0.4 eV larger for the magnetic ground state (AFM-Néel). Additionally, the curvature of the bands near the band edges is significantly affected by the magnetic state. The key property that defines the curvature of the bands is effective mass, that can be determined from transport measurements. We found that the effective masses strongly depend on the magnetic configuration. Namely, the smaller masses are obtained for FM state than corresponding quantities obtained for AFM configurations. Regarding various AFM arrangement of spins, the effective mass of holes for AFM-Néel are up to 40% larger than for AFM-s arrangement of spins. Overall, our results expose that the holes are less mobile carriers than the electrons independently of the magnetic ordering. Interestingly, our result unveil that for magnetic states that are incommensurate with the primitive structural cell, the in-plane components of the effective mass tensor exhibit anisotropic behaviour.

In the case of optical properties, we have shown in **[H4]** that the exciton binding energies at band edges are moderately dependent on the magnetic state. Notably, regarding the various AFM states, theirs transition are optically allowed (non-zero oscillator strength) exhibiting linear polarization of light. The type of the polarization of light de-

pends on the AFM state. Consequently, the AFM ordering of monolayer samples can be inferred indirectly using different polarization of light.

In contrast to the interlayer magnetism described above, the influence of intraleyer magnetism on selected physical properties have been explored in paper **[H8]**. Notably, in this work, we unveil that interlayer magnetic ordering strongly affects the electronic structure along high symmetry line of $\Gamma - Z$ in k-space, resulting in significant splitting of the conduction bands for FM ordering of spins at adjacent layers, whereas for A-AFM the bands are spin degenerated. Additionally, the character of the band gap from direct to indirect is altered upon the change of A-AFM to FM phase between adjacent layers. Regarding the vibrational properties, we have pinpoint the phonon modes which are sensitive to the interlayer magnetic ordering. Explicitly, in-plane phonon modes (B_{2g}, B_{2g}) are sensitive to the interlayer magnetic ordering, and can be regarded as a magnetic markers of interlayer magnetic ordering, while the out-of plane mode A_g are intact to the change of the out-of plane arrangement of the spins. In particular, the calculated increase in splitting between B_{2g} and B_{2g} obtained for FM compared to A-AFM correlates well with the increase of B_{2g}/B_{2g} splitting across the Néel temperature obtained from Raman measurements.

CHAPTER 5

Presentation of significant scientific activity carried out at more than one university.

After completing my PhD, I hold a two years post-doc position in a theoretical research group of Prof. J. Majewski, where I examined the properties of 2D materials crafted to metallic surfaces. Since 2019, I have started establishing a theoretical group specializing in first-principles calculations of nanomaterials. In this regard, I have launched broad collaboration with researchers working at national universities such as Warsaw University of Technology **(WUT)**, Wrocław University of Science and Technology **(PWr)**, International Centre for Interfacing Magnetism and Superconductivity with Topological Matter, Institute of Physics, Polish Academy of Sciences **MagTop (IF PAN)**, as well as at international institutions including **Technion** (Israel), University of Regensburg **UR**(Germany), **RWTH** Aachen University (Germany), University of Arkansas **UARK** (USA).

In particular, since 2019 I have been actively collaborating with experimental group of Prof. Agnieszka M. Jastrzębska from *Faculty of Materials Science and Engineering* **(WUT)** in the area of MXenes and newly emerged MBenes materials. Starting from 2020 we are leading a joint project (OPUS 18 started in 2020, consortium). This collaboration resulted in 8 common papers, including 3 review papers, among others *Adv. Materials* (IF=30), *Adv. Funct. Materials* (IF=19).

Regarding optical and mechanical properties of layered crystals, I intensively collaborate with the experimental group led by Prof. Robert Kudrawiec (**PWr**, started in 2020). Our collaboration resulted in 3 common papers. I am regularly invited to give seminar lectures and discuss research results at the Faculty of Fundamental Technological Problems in Wroclaw. We actively exchange the scientific knowledge by training the students within internships (Szymon Kałuza, Miłosz Rybak). I am currently co-promoter of a doctoral student (Miłosz Rybak), and Dr. Tomasz Wozniak (PWr) is a PI of SONATINA project (NCN) conducted at Faculty of Physics (UW) under my supervision.

In respect to various opto-electronic properties of 2D magnets, I actively collaborate with experimental group led by: Prof. Efrat Lifshitz (3 common publications, **Technion, Israel**); Prof. Marcus Morgenstern (electronic properties, 1 publication - ARPES measurements, **RWTH Aachen**), Prof. Jin Hu (1 publication, magnetic measurements, of alloys, **UARK, USA**).

In all aforementioned experimental collaborations we are the only theoretical group that is responsible for providing reliable physical explanation and shed light into physical mechanism of the observed experimental findings.

Regarding theoretical collaboration in the field of opto-electronics and spintronics, I actively collaborate with the group of Prof. J. Fabian (**UR, Germany**, effective models, excitonic properties of layered materials, 2 common papers) and theoretical team of Prof. Carmine Autieri (**MagTop, IF PAN**, model Hamiltonians, 3 common papers). Below, I listed other collaborations:
newly emerged collaborations: (Researcher, Institute, common research topic):

- Dr. Oleksander Pylypovskyi, (**HZDR** Germany, role of magnetic dipolar interactions in 2D magnetic crystals);
- Prof. Karol Szałowski (**University of Łódz (UŁ)**, charged density waves in heterolayers consisting MPX_3 materials);
- Dr. Andrea Leon (**Pontifical University Catholic of Chile**, magnetic properties of mixed 2D magnetic crystals from first principles);
- Dr. Mateusz Wlazło (**Ensamble**^{3} Center of Excellence (Warsaw), vibrational properties of $CrPS_4$ *ab inito* study

Past collaborations (Researcher, Institute, collaboration in years, no. of common papers):

- Dr. J. Kunstmann (TU Dresden, Germany, 2019-2021, 1 publication)
- Dr. S. Prucnal and Prof. Prof. Shenpianq Zhou (**HZDR** Germany, 2018-2021, 3 papers)
- Prof. P. Płochocka (**LNCMI** Toulouse, 2017-2018, 1 paper)

Other scientific activities during the period 2017-2023 (after completion of PhD) are summarized below:

Scientific collaboration within the research projects

- 10.2023 -10.2025, SONATINA project conducted at Faculty of Physics UW, PI: Dr Tomasz Woźniak: **(PWr Wrocław)**; founding agency: National Science Center in Poland (2023/48/C/ST3/00309),

- 07.2020 - 07.2024, OPUS 18, consortium - cooperation of two entities: **Faculty of Materials Science and Engineering, Warsaw University of Technology (PW) and Faculty of Physics (UW)**; founding agency: National Science Center in Poland (2019/35/B/ST5/02538), leader PW: dr. inż. hab. A. M. Jastrzębska; Principle Investigator (PI) on behalf of the partner - dr. Magdalena Popielska (Birowska),

- 08.2017 - 02.2021, SONATA 12 project, founding agency: National Science Center in Poland (UMO-2016/23/D/ST3/03446), PI: dr. Magdalena Popielska (Birowska), collaboration with international scientific groups: Prof. Shenpianq Zhou **(HZDR, Germany)**, Prof. Paulina Plochocka **(LNCMI Toulouse, France)**, Prof. Jaroslav Fabian **(UR, Germany)**.

- 12.2014 – 09.2017, HARMONIA V, NCN (2013/10/M/ST3/00793) within the framework of international cooperation with Prof. Claudia Draxl **(Humboldt University in Berlin)**. PI: Prof. dr hab. J. A. Majewski (Faculty of Physics, UW); participation in research (*post-doc position*) - dr M. Popielska.

Research experience gained abroad:

Short research stays after completing PhD:

- **March 2022** (1 week), University of Regenbsburg, Faculty of Physics (Germany), research group **Prof. Jaroslava Fabiana, Dr. Paulo E. Faria Junior**
- **February 2019** & **April 2019** (2 weeks), Technische Univeristat (TU) Dresden, Germany; research group: **Prof. Thomas Heine, Dr. Jens Kunstmann**;
- **April 2019**, Departments of the Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany; **Prof. Shengqiang Zhou, Dr. S. Prucnal**;
- **April 2019** (1 week), Austria, Institute of Semiconductor & Solid State Physics, Johannes Kepler Universitat (JKU) Linz, Austria; reaserch group: **Prof. Alberta Bonanni.**

CHAPTER 6

Presentation of teaching and organizational achievements as well as achievements in popularization of science

Teaching activities

I conducted following lectures:

- **(Spring Semester 2022)** - (1100-4INZ21) 45h, **"Modeling of nanostructures and materials"** in English, Faculty of Physics, UW, 2 cycle programme;
- **(Fall Semesters: 2020, 2021, 2022)** - (1100-3INZ12) 30h, **"Modelowanie Nanostruktur"** in Polish, Faculty of Physics, UW, mandatory course lecture for Nanoengineering, 1^{st} cycle, 3^{rd} year courses Nanostructures Engineering programme;

and practical courses:

- **(Spring semester 2021)** (1100-4INZ21) 45h, **"Modelling of nanostructures and materials"** in English, Faculty of Physics, UW, 2 cycle programme;
- **(Fall Semesters: 2019, 2020, 2021)** (1100-3INZ12) 45h, **"Modelowanie Nanostruktur"** in Polish, using Python 3.0, undergraduate course, Faculty of Physics, UW;
- **(Fall Semesters: 2014)** - (1100-3INZ12) 45h, **"Modelowanie Nanostruktur"** in Polish, in Mathematica, Faculty of Physics, UW;
- **(September 2013)** - **„START II - Quantum Mechanics"** , graduate course, Faculty of Physics, University of Warsaw;
- **(Fall semester 2010)** - (1100-1INZ04) 30h, **„Algebra and Geometry"**, undergraduate course, Faculty of Physics, University of Warsaw (UW);
- **(Fall semester 2010)** (1100-2INZ13) 45h, **"Programming and Numerical Methods"**, in Fortran 90, undergraduate course, Faculty of Physics, University of Warsaw;
- **(Spring semester 2010)** (1100-1015) 45h, **„Mathematics II"**, undergraduate course, Faculty of Physics, University of Warsaw, **(Dean's award)**

I was a supervisor of 3 master students and 3 bachelor's students, and co-supervisor of 3 PhD students, including two ongoing ones. A detailed list of the students is summarized below:

Ph.D. thesis Supervision:

- **3rd October 2022** - Ph.D. thesis defense of ***Maciej M. Marchwiany***, Faculty of Physics, University of Warsaw,*"Description of properties of low-dimensional nanostructures by machine learning algorithms"*, **(co-supervisor)**.
- (Ongoing doctoral studies) ***Miłosz Rybak*** - Ph.D. studies started in Oct. 2022 at Department of Semiconductor Materials Engineering Faculty of Fundamental Problems of Technology Wrocław University of Science and Technology, the title of doctoral thesis is: *Modelling of the 2D magnetic materials using ab intio methods*, **(co-supervisor)**.
- (Ongoing doctoral studies) ***Varun G. Nair*** - Ph.D. studies started in January 2021 at Warsaw University of Technology, Faculty of Materials Science and Engineering, the title of doctoral thesis is: *Modelling of the MXenes and MBenes materials using density functional theory and machine learning approach*, **(co-supervisor)**.

M.Sc. & **B.Sc. thesis Supervision:**

- **27th February 2023** - Bachelor's thesis defense of ***Marek Sokołowski***, Faculty of Physics, University of Warsaw, *"Stability studies of novel 2D alloys M_xB_{1-x} using ab initio methods and Machine Learning approach"*,

- **21th December 2022** - Bachelor's thesis defense of ***Aleksandra Skolasińska***, Faculty of Physics, University of Warsaw, "Study of the dielectric properties of MPX_3 family using ab initio methods",
- **22th July 2022** - Master's thesis defense of ***Kamila Kotur***, Faculty of Physics, University of Warsaw, *"Tuning the magnetic properties upon non-magnetic substitution in MPX_3 (M = Ni, Mn; X = S, Se) systems"*,
- **12th July 2022** - Master's thesis defense of ***Miłosz Rybak***, Department of Semiconductor Materials Engineering Faculty of Fundamental Problems of Technology, Wroclaw University of Science and Technology, *"Badania ab initio dwuwymiarowych magnetyków z rodziny MPX_3."*, ("Ab initio studies of two-dimensional magnets of MPX3 compounds"),
- **8th October 2020** - Bachelor's thesis defense of ***Kamila Kotur***, Faculty of Physics, University of Warsaw, *"Theoretical studies of electronic properties of the $NiPS_3/FePS_3$ layered heterostructure"*
- **10th August 2020** - Master's thesis defense of ***Tomasz Necio***, Faculty of Physics, University of Warsaw, *"An ab initio study of the energetic, structural, and magnetic properties of the $NiPS_3$/graphene heterostructure"*.

Reviews of bachelor's and master's theses

- **september 2023** - bachelor thesis, **Marta Przybył**, *Coherent charge and spin transport in lateral structures of transition metal carbides - MXenes*,
- **september 2022** - master thesis, **Jan Kołodziejczyk**, *Stability, electronic structure, and thermoelectric properties of functionalized 2D molybdenum nitrides (MXenes)*;
- **september 2020** - bachelor thesis, **Dominik Suwała**, *Simulations of spin-orbit splitting in elemental 2D materials of group IV and their derivatives*;
- **december 2019** - master thesis, **Przemysław Zieliński**, *"Tight-binding method for electronic states of non-periodic carbon nanostructures"*;
- **september 2019** - bachelor thesis, **Adam Ćwilich**, *"Modeling of quantum tunneling effects in nitride heterostructures"*;
- **may 2017** - bachelor thesis, **Maciej Celuch**, *"Surface states model implementation of topological crystalline insulators"*;
- **september 2016** - master thesis, **Łukasz Gładczuk**, *"Electronic Structure of Two-dimensional Alloys of group IV Elements"*.

Organizational activities

Participation in committees as:

- Secretary of the department committee in 8 distinctive commissions regarding promotion to the position of Associate Professor held in the years: 2021-2023.
- Secretary of 2 department committees for the competition for the position of assistant professor of teaching and research in 2022 and 2023.
- Member of the Council of the Institute of Theoretical Physics from 2020 to 2024;
- Member of the Faculty Council in the previous term.
- Member of *American Chemical Society* from 2020 to 2022.
- Member of Polish Physical Society from 2019 to 2020.

Popularization activities

I was invited to give a lecture in private company **Astra Zeneca R&D** Poland, **14^{th} July 2021**: *"Exploration of the properties of 2D materials using Machine Learning method"*, M. Birowska. In addition, I was giving lectures during the **summer school**, organised by Interdisciplinary Center for Mathematical and Computer Modeling (ICM) at the University of Warsaw during **28.06 - 09.07.2021**, entitled: *"Applications of advanced data processing in life sciences"*.

Developed Software:
Supercell-core: A useful tool to generate an optimal supercell for vertically stacked nanomaterials
AIP Advances 10, 105105 (2020)
Supercell-core download
Graphical User Interface of Supercell-core: GUI

CHAPTER 7

Other information about her professional career, which she deems important.

Reviews of articles for scientific journals

I have reviewed 20 scientific articles in 2019-2023:

- **Nature Communications** (IF=17.7) → 1 review in 2023.
- **Physical Review B** (IF=3.9) → 2 reviews in 2023, 2 reviews in 2021, 4 reviews in 2020.
- **Applied Sciences** (IF=2.838)→ 1 review in 2020.
- **Journal of Physics: Condensed Matter** (IF=2.7)→ 1 review in 2020.
- **2D Materials** (IF=6.9) → 2 reviews in 2019
- **Journal of Raman Spectroscopy** (IF=2.7) → 1 review in 2019.
- **Journal of Physics D: Applied Physics** (IF=3.4) → 2 reviews in 2020.
- **Physical Chemistry Chemical Physics** (IF=3.9)→ 2 reviews in 2019.
- **FlatChem** (IF=5.8) → 1 review in 2023.
- **Materials** (IF=3.7) → 1 review in 2019.

Team building and management skills

Members of the research team (August 2023):

- *Postdoc:* - **Dr Subrahmanyam Bandaru**, employment within the project OPUS 18;
- *2 PHd's*: **Miłosz Rybak** (participation in the project IDUBB), **Varun G. Nair** (participation in the project OPUS 18).
- **Dr. Mateusz Wlazło** is conducting research tasks at the Faculty of Physics (02.2023 -12.2023) within the framework of the agreement between ENSEMBLE3 Ltd. and Univeristy of Warsaw. **Mr. Szymon Kałuża**, a student of Faculty of Fundamental Problems of Technology Wrocław University of Science and Technology, is carrying out a month-long student internship.
- Former team members (*alumni*): **MSc Tomasz Necio** (2 years, participated in the SONATA project), **MSc Kamila Kotur** (3 years, participated in the SONATA project), **B.S. Marek Sokołowski** (1 year, participated in the OPUS 18 project).

I took part in a in a course regarding professional competence entitled: *"Challenges of leadership"* within the framework of the Integrated Development Program (ZIP) on 14-15.09.2020.

Participation in conferences of team members (oral presentations and posters)

A list of scientific conferences of my research team in period 2018-2023. The person presenting the results is denoted in bold:

2023:

- ***E-MRS Fall Meeting 2023,*** 18-21 September 2023, Warsaw, Poland: **(oral presentation)**: *Review on thermoelectric properties of MXene-based structures and other 2D materials*, **S. Bandaru**, A.M. Jastrzębska, M. Birowska;
- ***36th European Conference on Surface Science***, 28.08-01.09.2023, Łódz, Poland, **(oral presentation)**: *Band gap engineering of two-dimensional ScB MBene*, **S. Bandaru** M. Birowska, A. M. Jastrzębska;
- ***51th International School*** & ***Conference on the Physics of Semiconductors "Jaszowiec 2023"***, 17-23 June, Szczyrk, Poland; **(oral presentation)**: **(poster)**: *Tunable valley splitting in 2D MPX_3 crystals.*, **M. Rybak**, M. Birowska; **(poster)**: *Optical markers of magnetic phase transition in layered CrSBr* , **M. Rybak**, W. Linhart, M. Birowska, P. Scharoch, R. Kudrawiec;

2022:

- ***50th International School*** & ***Conference on the Physics of Semiconductors "Jaszowiec 2022"***, 4-10 June, Szczyrk, Poland; **(poster)**: *Theoretical studies of the optical properties of MPX_3 (X=S,Se) -2D magnetic crystals*; **M. Rybak**, P. E. Faria Junior, T. Wozniak, P. Scharoch, and M. Birowska;
- ***E-MRS Spring Meeting 2022***, 30 May - 3 June, Virtual Conference **(oral presentation)**: *Excellent excitonic properties and non-zero valley splitting in 2D antiferromagnetic MPX_3 crystals*; **M. Rybak**, P. E. Faria Junior, T. Wozniak, P. Scharoch, J. Fabian, J.Kunstmann and M. Birowska.

2021

- ***49th International School*** & ***Conference on the Physics of Semiconductors "Jaszowiec 2021"***, 1-10 September: **(poster)** *The influence of the magnetic ordering on the electronic properties of bilayer $NiPS_3$ – an ab inito study of vdW heterostructure*; **K. Kotur**, M. Birowska; **(poster)**: *Optical properties of transition metal trichalcogenides MPX_3: a first principle study of 2D magnets*; **M. Rybak**, T. Woźniak, P. F. Junior, P. Scharoch, M. Birowska; **(poster)**: *Dielectric properties of transition metal trichalcogenides MPX_3*, A. Skolasińska, M. Birowska; **(poster)**: *Structural search and stability prediction of new M_xB_{1-x} phases based on ab inito calculations and Machine Learning Methods*, **M. Sokołowski**, M. Marchwiany, A. M. Jastrzębska and M. Birowska; **(poster)**: *Exploring Electronic Properties of Functionalized 2D MBenes -Graphene Like 2D Boron Sheets*, **V.G. Nair**, K. Kotur, A.M. Jastrzębska and M. Birowska.

- ***Intermag 2021, 26-30 April 2021***, Virtual Conference **(oral presentation)**: *The Impact of the Intralayer and Interlayer Magnetism on the Electronic Properties of vdW Heterostructure $NiPS_3/FePS_3$ – a Theoretical Approach,* **K. Kotur** and M. Birowska.

- ***33^{rd} Workshop on Recent Developments in Electronic Structure (ES21)***, 12-15 July 2021; **(poster)**: *First-principles study of magnetic bilayer of $NiPS_3/FePS_3$*, **K. Kotur** and M. Birowska.

- ***MiniModes 2021***, Chęciny, Polska, *Structural search and stability prediction of new M_xB_{1-x} phases based on ab initio calculations and Machine Learning Methods*, **M. Sokołowski**, M. Birowska.

2019:

- E-MRS Fall Meeting 2019, 16-19 September 2019, Warsaw, Poland: **(oral presentation)**: *Ab initio study of mixed manganese nickel phosphorus trichalcogenides- 2D layered materials*, **Aleksandra Jankowska** and M. Birowska; **(poster)**: *The impact of the different stacking configurations of the monolayer of $NiPS_3$ and graphene layer on the electronic properties of $NiPS_3$ structure*, **Tomasz Necio** and M. Birowska.

Scholarships & Awards:

- 2013 - *Ministry of Science and Higher Education* scholarship for outstanding, achievement in period 2012/2013,
- 2012, 2013 Scholarships for the best doctoral students at UW in period of 2011/2012/; 2012/2013,
- 2010/2011 *Modern University* Scholarship, co-financed by the European Union with the European Social Fund (ESF), Operational Programme Human Capital, Warsaw,
- 03 Feb 2010, Dean's Award for the conduct of Physics teaching at the UW,
- 2009 Mazovia scholarships for PhD students.

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Magdalena Popielska