Project Title: **Pressure Induced Proximity Effects in FeI2 Monolayer**
Project Acronym: **PIPEFeM**
Applicant Name: **Bc. Martin Lukáč**

Project summary [600 words]:
In recent years with better equipment, synthetization of new monolayer materials opened research of new quantum effects in 2D materials. Here, we propose theoretical study based on first principle DFT (Density Field Theory) calculations of different phases of FeI2 monolayer coated in graphene. Our study can enhance the understanding of phase stability affected by proximity effects of graphene and in future can lead to creating sensors with longer stability and higher effectiveness.

EXCELLENCE

Present state of subject [800 words]:
From 1970s there is lot of experimental studies about FeI2 bulk. These studies describe FeI2 as antiferromagnetic material crystalized in trigonal crystal system with the space group P $\overline{3}m1$.
Recent theoretical studies of FeI2 monolayer suggest, that there is change in magnetic phase to half-metal, which means that electrons with only one direction of magnetization contribute to the conductivity of this monolayer. These results open new possibilities of its use in spintronic devices.
Lately, new experimental findings obtained from STM (Scanning Tunneling Microscopy) suggest, that different phases are observed in FeI2 monolayer coated in graphene. This phenomenon is accompanied by weird shape of hysteresis loop of magnetization called Wasp-waisted hysteresis. These results suggest that different FeI2 phases have different magnetic configurations which lead to this occurrence.

Scientific goal(s) [400 words];
We propose theoretical study of different deformations of FeI2 monolayer found with STM measurement. The task is to determine the magnetic phases of these deformations with goal of understanding of wasp-waisted hysteresis loop. To confirm our theory we need to confirm, that graphene induced proximity effects are responsible for stability of these deformations.
Secondly our goal is to calculate ground state and then corresponding band structures to determine electrical properties of these deformations.

Research methodology [500 words]:
For out theoretical study we will use ab initio DFT calculations contained in program Quantum Espresso (QE), which uses plane wave basis sets and pseudopotentials. Basic package *pwscf* solves self-consistent Kohn-Sham equations, obtained for periodic solid crystal.
To find ground states of different phases we will use Relax package, which calculate scf (self-consistent field) equations for every step of relaxation and then calculate force acting on the crystal and adjust new geometry accordingly to minimize the pressure on unit cell.
For calculating Hubbard U parameter, we are going to use DFPT (density functional perturbation theory), by constructing the response of the system to a localized perturbation through a series of independent monochromatic perturbations to the primitive cell.
To calculate exchange parameters, we will use Wannier package in QE. Firstly, we wannierize our band structure and then we calculate with program TB2J exchange parameters.

IMPACT OF RESEARCH

Enhancing the potential and future career prospects [400 words]:

Theoretical approach, based on studying electrical properties of materials using first principle DFT approach, has in recent years gained in popularity, because of new more powerful computational devices. This method of theoretical research is expected to be grow even more soon, with prospect of career opportunities in material modelling.

This project will enhance practical knowledge of using programs Quantum Espresso, Vesta and xCrysden, which are commonly used in material modelling and theoretical understanding of phenomena such as phase transition in 2D crystals, proximity effects of bilayers and behavior of 2D materials in global.

Exploitation and dissemination of results [400 words]:

Results are expected to be published as article in Physics Letters, Section A as cooperation with experimental Condensed Matter group in University Pavol Jozef Safarik in Kosice.

Additionally, useful results will be used in further semiconductor research in the class of Iodide semiconductors with possible use in real devices.

IMPLEMENTATION

Work plan and tasks [600 words]:

We can divide our tasks into 3 groups with start from July 2024 to June 2025. In the first part we will deal only with undeformed FeI2 monolayer (M1):

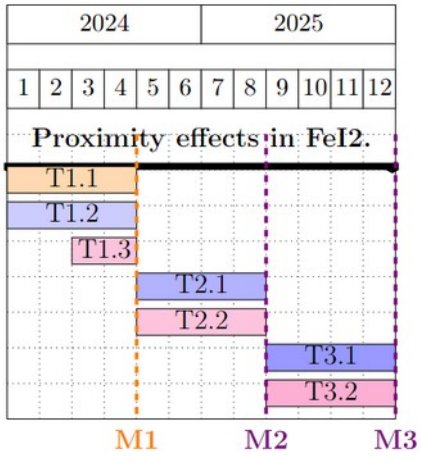
1. Calculation of ground state of FeI2 monolayer and determination of magnetic phase. (T1.1)
2. Calculation of Hubbard parameter U without and with spin-orbit coupling for undeformed (T1.2)
3. Band structure of FeI2 monolayer. (T1.3)

In next part we are going to try to simulate results obtained from STM and examine deformed phases of FeI2 monolayer (M2):

4. Creation of input files of deformed FeI2 phases from STM. (T2.1)
5. Find ground state of deformed phases and understand proximity effects of graphene. (T2.2)

In last part we are going to examine magnetic properties of undeformed and deformed phases of FeI2 monolayer (M3):

6. Calculate exchange parameters for all relaxed structures. (T3.1)
7. Model magnetic hysteresis loop based on exchange parameters. (T3.2)



For acronym use a single word to abbreviate your project. Maximally expected number of words for each sections are given.

Risk management [400 words]:

In case of problems with calculating exchange parameters with spin-orbit coupling, we will use program OpenMX.

If problems emerge with modelling the proximity effects of graphene, because of large unit-cell, we can simplify problem with substituting graphene with charged plates of same charge.