Werner Heisenberg, a renowned physicist, stated in 1924 that only d and f orbitals can lead to magnetism. Nevertheless, after 70 years it has been shown, both theoretically and experimentally, that ferromagnetism (FM) can arise in s and p electron compounds [1]. Due to the lack of d-orbital electrons it is called d0 magnetism. FM has been observed in molecular systems, even in room temperature [2]. In solid state the phenomena induce non vanishing spin polarization and exhibits two flavors: (a) "local" as high spin (HS) states of defects, eg., cation vacancies in GaP [3] ; (b) "global" as collective magnetism in the systems, eg., in II-VI oxides, III-V nitrides or material systems based on C where spin moments are due to defects or dopants from second row, like C, N, O [4,5]. The stability of HS state, as well as the resultant magnetism, depends on a number of factors. It is correlated with the spin polarization of 2p electrons of light atoms, like C, O, N.

The aim of this project is to investigate using density functional theory (DFT) the magnetic interaction of magnetic centers in GaN, BN, SiC and ZnO. Both magnetic and electronic properties of cation vacancies, divacancies, vacancy-the second row dopant are to be researched.
The majority of effort will be dedicated to bulk materials. Quantum wires and quantum dots will also be covered.

Correct desciption of electronic structure is of great significance to the project. Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA) have the drawback of the underestimation of the bandgap, Egap, of semiconductors. Correct bandgap values can be calculated within semiempirical LDA+U (GGA+U) approach that supplants LDA (GGA) with +U correction
applied on the selected orbitals [6]. The project aims to investigate the validity of +U corrections applied on p orbitals.

The proposed problems to be covered in the project are the continuation of the past work which resulted in a number of important results [1, 7-9].
The analysis of magnetism in IIA-V compounds, as well as determination of electronic and spin structure of III-V nitrides and II-VI oxides, allowed to
identify the mechanism responsible for magnetic properties in those systems. Both, spin polarization of bulk materials and magnetic moments are coupled with the spin polarization
of p orbitals of atoms consituting the material, or as in case of vacancy with the spin polarization of p orbitals forming the broken bonds.

The proposed project aims to comprehend the abovementioned interdependancies: electronic and spin structure of defects, the role of localization of wave functions, the stability of collective
magnetism. On the other hand, the topic is also important from the application perspective, namely VN complex in diamond and vacancy or divacancy in SiC.

The possible applications of localized spins of electrons in the context of secure communication and quantum computing invoked alot interest among researchers working with diamond and silicon.
In particular, vacancy-N atom complex (VN) in diamond and P dopant in Si demonstrated astonishing spin coherence (ie., lifetime of spin state) [14]. The investigations of single spins localized on the defects
are not restricted to those complexes. It has been shown recently that defects in SiC exhibit milliseconds time spin coherence. Hence, the interest of the defects in SiC.
One of the things to be performed in the project is the comparison of electronic and magnetic properties of VN in diamond with the the vacancy - O atom complex, VO, in GaN, InGaN, and BN and also
vacancy and other defect complexes in SiC. All those for the sake of finding attractive candidates in quantum spintronics. The major effort will come to the determination of
electronic strucure of defects, ie., the introduced defect levels, as well as spin state as a function of charge state.

In last decade, a lot of attention was put to the investigation of semiconductors doped with transition metals, especially GaN. The correct description of p(N) orbitals is important, and p orbitals of anions like oxygen and nitrogen play a crucial role in the magnetism, e.g. of
GaN:Mn and GaN:Fe. It harks back sp-d hybridization that is the basis of semiconductor magnetism coupling the magntetic properties with the valence electrons,
which are mainly built with p orbitals of anions. The exact impact of anions comprising the material matrix has eluded a complete treatment from first principles.
The project will cover the investigation of the role of anions for ZnO doped with Cu. My past investigations during PdD studies and after covered the magnetism of II-V compounds, cation vacancies in III-V, II-VI and I-IV compounds, and transition metal doped compounds. The proposed project extends those investigations in the area of spin states of vacancies, vacancy-dopant complexes, Cu dopants and coupling within semiconductors.
I want to prove that the strong polarization of p orbitals of light atoms stands behind magnetic phonomena in all the above cases. This integrating approach should find its place in the theory of magnetism in
semiconductors.

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