# Fariba Kafikang

*Curriculum Vitae*

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## Education

2007–2012 **B.Sc. in Physics**, Payame Noor University of Mashhad, Mashhad, Iran
(Iranian GPA: 13.99/20.00)-(Converted GPA: 2.46/4)

2013–2017 **M.Sc. in Physics**, Payame Noor University of Mashhad, Mashhad, Iran
(Iranian GPA: 13.99/20.00)-(Converted GPA: 2.46/4)

2021–2024 **Ph.D. in Nuclear Physics**, Shahrood University of Technology, Shahrood, Iran
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## Experience

2011–2016 **TA**, *Payame Noor University Mashhad*, Mashhad, Iran

2018–2021 **Advisor of M.Sc Thesis**, *Payame Noor University Mashhad*, Mashhad, Iran

2022–2024 **TA**, *Shahrood University of Technology*, Shahrood, Iran

## Skills

Programming Languages: Python, C++

Tools: Git, Linux

Software: Wien2k, Quantum Espresso, Mathematica, Origin, BoltzTrap

## Projects

M. Sc **First principle study of the optical and vibrational properties of mono-layer molybdenum disulfide under Strain** – In this research, the electronic, optical and phononic properties of $MoS_2$ in the Bulk and Monolayer state without strain, under pressure and tension were investigated using quantum Espresso and Wien2k computing packages based on density functional theory.

Ph.D **Analytical investigation of white dwarfs by $\kappa$-deformed quantum mechanics** – In this treatise, we discuss how to obtain this special algebra from quantum mechanics, then we obtain the Schrödinger equation and the relativity equation, we solve this equation for a group of special interactions and reduce it to N particles. We generalize and using the system of fermions, we obtain the spectrum and special values of the particle for it. After introducing deformation formalism, we study trigonometric, logarithmic functions, weight functions, and other properties in the presence of deformation formalism. With the existence of the parameter in this formalism, we can apply it to theoretical models that have some uncertain parameters, and we can determine these parameters by fitting or scanning. Also, using this deformation formalism, we calculate the thermodynamic properties in the harmonic oscillator problem and show that can be used as a parameter to adjust the thermodynamic properties. Since in white dwarfs, the pressure caused by convection and gravity are equal, we have calculated and checked the radius of the white dwarf in different densities, which is in good agreement with the results of others.

## Languages

Persian Native

English Fluent

## Professional Interest

Quantum mechanics

Field Theory, Gravity

Density Functional Theory

Computational Physics

Condense Matter Physics

Optical and Vibrational Properties in Solids

## Articles

2017 **Optical Properties of $MoS_2$ bulk and Monolayer under compressive and tensile strain: A First Principles Study** –( Journal of ELECTRONIC MATERIALS )– Knowledge of the optical properties under compressive and tensile strain is highly important in photoelectron devices and the semiconductor industry. In this work, optical properties of bulk and monolayer $MoS_2$ under compressive and tensile strains are investigated by means of density functional theory. The dielectric tensor is derived within the random phase approximation. Calculations indicate that unstrained two-dimensional and bulk $MoS_2$ lead to semiconductors with the gaps of 1.64 eV and 0.84 eV, respectively, whereas the change in the value of the gap by applying tensile or compressive strain depends on the nature of strains. Dielectric function, absorption coefficient, reflectivity, energy loss and the refraction index of the strained and unstrained systems are studied for both parallel (E||x) and perpendicular (E||z) applied electric field polarizations, which are very sensitive to the type and amount of strains.

2019 **Effects of strain on the electronic and optical properties of MgO (111) nanoshee** – (Optik) – High optical transparency, thermal and thermodynamic stabilities, low dielectric constant and refractive index of MgO are promising for different applications of this material. In this work the electronic and optical properties of MgO (111) nanosheet under compressive and tensile strain were investigated by density functional theory (DFT). The results showed that the band gap of MgO nanosheet decreased from 3.45 to 2.16 eV when tensile strain of s = 15% was applied on the lattice parameter of MgO and increased to 4.05 eV by means of compressive strain of s=- 15%. The optical parameters such as real and imaginary part of dielectric function, reflectivity, refraction, extinction coefficient and energy loss and their alterations under applied strain were studied. Position of plasmon peak was changed in linear pattern as a function of applied strain from s=−15% to 15%.

2019 **Electronic, optical, vibrational and EFG properties of tetragonal BaTiO3 under pressure: By first-principles study** – (Chinese Journal of Physics) – The First principles study on structural, electronic, Electron Field Gradient (EFG), optical and vibrational properties of tetragonal BaTiO3 have been done in the framework of Density Functional Theory (DFT). Obtained structural properties are in agreement with others and also, the electronic study shows that the tetragonal BaTiO3 has an indirect energy gap (Eg) about 1.864eV by GGA and 2.6eV by GGA-mbj at equilibrium state and by decreasing pressure the Eg shifts toward small value. By increasing pressure to 31.479GPa the EFG decrease for O atom and increase for Ba and Ti atoms that is a sign to piezoelectric property for tetragonal BaTiO3. The optical parameters under pressure, such as real and imaginary dielectric function, Loss function, reflection index, absorption coefficient, conductivity and reflection were studied. Moreover, by applying hydrostatic pressure the real part of the dielectric constant roots shift towards higher energy and the energy loss and absorption peak intensity were reduced. Finally lattice vibration survey indicates the stability of tetragonal BaTiO3 under pressure.

2020 **Thermoelectric properties of InN graphene like nanosheet: A frst principle study** – (Superlattices and Microstructures) – In this work, the electronic and thermoelectric properties of the graphene-like monolayer of InN were investigated by utilizing Wien2k and BoltzTrap codes considering PBE-GGA and mBJ potentials. The bandgap of InN monolayer was estimated at 0.72 and 0.98 eV by GGA and mBJ, respectively. The thermoelectric properties of the Seebeck coefficient, electrical conductivity, electronic thermal conductivity, electronic specific heat, power factor and figure of merit were investigated in terms of temperature and potential energy. The figure of merit which describes the quality of material for thermoelectric applications was estimated at 0.92 for $\mu = -0.11$ and 0.93 for $\mu = 0.13$ with respect to $\mu_0$ at T =300 by GGA and mBJ respectively which are reasonable for practical applications. Also, it has been found that the figure of merit of InN monolayer remains close to the mentioned values at higher temperatures up to 800 K.

2020 **First principles investigation of vibrational, electronic and optical properties of graphene-like boron carbide** – (Solid State Communications) –In this study, the vibrational, electronic and optical properties of graphene-like structure of boron carbide were investigated by density functional theory and the results were compared to the calculated properties of graphene. By investigating the phonon dispersions and vibrational properties, the BC monolayer found stable and revealed lower group velocity and higher specific heat capacity than graphene. In contrast to graphene, metallic characteristic of graphene-like boron carbide was confirmed by analyzing the total density of states and band structure which could be responsible for the observed different optical properties compared to graphene particularly at low energy region of electromagnetic waves spectrum.

2020 **Stability and thermoelectric properties of the MgO monolayers under tensile and compressive strain** – (Physica E: Low-dimensional Systems and Nanostructure)In this study, the stability and thermoelectric properties of MgO (111) and (100) monolayers under compressive and tensile strain were investigated by density functional theory. The flat MgO (111) revealed to be stable against a biaxial and uniaxial tensile strain of up to $\epsilon = 15\%$ and compressive strain of up to $\epsilon = -2\%$ for biaxial strain and -5% for uniaxial strain. The rumbled MgO (100) showed stability for the only tensile strain of up to 8%. The thermoelectric properties of the MgO monolayers predict the figure of merit of about unity in both n- and p-type doping regions which found to be promising for practical application of MgO monolayers in thermoelectric devices.

2022 **Two-dimensional quantum confinement effects on thermoelectric properties of MgO monolayers: A first principle study** – (Superlattices and Microstructures) –In this paper, the thermoelectric properties of magnesium oxide in the bulk and monolayer (ML) phases in the two facets of (100) and (111) have been calculated and compared by using density functional theory (DFT) and Boltzmann theory. The electronic band structure calculations of bulk and monolayers of MgO indicate that the band gap for bulk and MgO(100) ML is direct, and indirect for MgO(111) ML K-to $\Gamma$-point. The estimated band gaps are in good agreement with other theoretical and experimental works. Due to the quantum confinement effects, two small peaks are observed in the n-doping region of the room temperature Seebeck coefficients of the monolayers which are not present in the bulk structure.

2023 **Radius of the white dwarf according to Fermi energy in a -deformed framework** – (The European Physical Journal Plus)In this article, the -deformation formalism, which is in the form of $e_\kappa(x) = (\sqrt{1+\kappa^2x^2}+\kappa x)^{1/\kappa}$, is investigated. Using the $\kappa$-deformation, the Fermi energy, for box problem with the Schr¨odinger equation, has been investigated and calculated. In addition, we calculated the internal energy and pressure, and also calculated the radius of the white dwarf with the pressure due to degeneracy and gravity.

2023 **Modified Lane-Emden Equation and Modified Jeans' Instability Based Gravity with Deviation** – (International Journal of Theoretical Physics) – In this paper, the gravity with a deviation is considered. Modification of the Lane-Emden equation and Jeans' instability condition is performed based on the gravity with a deviation. Some exact and numerical solutions are given for the modified Lane-Emden equation.

2024 **Investigation of the white dwarfs based on deformed Lane–Emden equation** – (Annals of Physics) – In this article, gravity is considered with deviation and we solved the Lane–Emden equation using this deviation, first, we calculated the pressure and potential due to gravity, and considering the density resulting from solving this equation, we obtained the radius of the white dwarf in different states. We obtained the ordinary cases when the deformation parameter goes to zero.

2026 **Effect of a q-deformed and modified Lane-Emden parameters on the radius of white dwarf** – (Annals of Physics) – In this work, we examine how q-deformation and modifications to the Lane–Emden parameter affect the radius of white dwarfs. We derive the electron Fermi energy in a three-dimensional box, then solve the classical and q-deformed Lane–Emden equations to obtain the stellar radius under various conditions. Our results show that q-deformed statistics alter the equilibrium structure and lead to deviations from standard predictions. When the deformation parameter vanishes, the ordinary cases are consistently recovered.

## References

**Prof. Hassan Hassanabadi** – My Ph.D thesis supervisor Faculty of Physics, Shahrood University of Technology, Shahrood, Iran.

**Prof. Filip Studnička** – Department of Physics, Faculty of Science, University of Hradec Králové, Rokitanského 62, 500 03 Hradec Králové, Czechia