JDD2023 :8-9 Mai 2023

Simulation of optoelectronic and photovoltaic properties of organic composites based on new conjugated copolymer MEH-PPV-P3HT for organic solar cell application

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Code : 463032 **Commission** :physique **Salle** :3

Mots clés : DFT, charge transfer, OSC, PCE

Abstract :

In this study, a new conjugated copolymer based on Poly(2-methoxy-5-(2-ethyl-hexyloxy)-1,4-phenylene-vinylene) (MEH-PPV) and poly(3-hexylthiophene) (P3HT) has been investigated. To predict the effect of the copolymerization between these two materials, DFT and TD-DFT calculations were utilized to determine the structural and optoelectronic properties. The obtained results show that there are two possible architectures of coupling between the two basic polymers. In addition, a hypothesis of rupture of conjugation of MEH-PPV and higher contribution of P3HT was discussed. Then, this copolymer has a low gap energy (in the order of 2.4 eV) which implies that it may be applied as an active layer in an organic solar cell. Thus, new organic composites have been modeled based on the MEH-PPV-P3HT copolymer as a donor material mixing with the PCBM as an acceptor material. The simulation of the photophysical and photovoltaic parameters of this composite was carried out. The obtained result shows that the addition of the PCBM improves the charge transfer process and reduces the gap energy to be in the order of 1.4 eV. Moreover, the copolymerization between the MEH-PPV and P3HT enhances the power conversion efficiency (PCE) from 3% to 5.2%.

JDD2023 :8-9 Mai 2023

Theoretical investigation of electronic and optical properties of a new D-π-A-π-D synthesized donor molecule for a new generation of fullerene-based bulk heterojunction (BHJ) for new organic solar cells application

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Code : 463523 **Commission** :physique **Salle** :3

Mots clés : dft, solar cells applications, organic material, charge transfer

Abstract :

In this study, a news SMi (i = 1–4) benzothiadiazole derivatives are designed and studied by the modification of the acceptor (A) ring. Theoretical calculations using DFT and TD-DFT methods, show the presence of an intramolecular charge transfer process from R molecules to SMi ones. Indeed, the calculated dipole moment variation (μCT) between the ground and the first excited state increases. Consequently, an improvement of the absorption in the visible part, and a reduction of the calculated optical band gap and the energy gap HOMO-LUMO are obtained. Furthermore, the calculated power conversion efficiency (PCE) factor of the bulk-heterojunction (BHJ) based on the investigated molecules (R and SMi, i = 1–4), as donor material and the fullerene (C60) as an acceptor one, increases drastically from 8% for R molecule to 13.5% for SM3 one according to Marks diagram.

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Effect of the capped matrix and geometric factors on linear and nonlinear optical properties in CdS/ZnSe core/shell quantum dots spheroid-shaped.

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Code : 463750 **Commission** :physique **Salle** :3

Mots clés : Intersubband transitions, QDs spheroid shaped, optical properties

Abstract :

In this study, we have numerically performed the linear and third order nonlinear optical properties of (CdS/ZnSe) prolate spheroidal core/shell quantum dot (SCSQD) capped in different dielectric matrices as PVC, PVA and SiO2. The Schrodinger equation has been resolved under the effective mass approximation (EMA) to calculate the energy states and corresponding wave function. Our results proved that the linear and nonlinear absorption coefficient and the refractive index change are sensitive by the geometric factors of the spheroidal quantum dots (QDs) shape and the surrounding matrix. When the eccentricity increases, the transitions energy decreases considerably and the resonance peak positions are red shifted. The suitable choice of the dielectric matrix and the geometrical size offers the possibility of tuning the optical properties of the QDs which are important of optoelectronic and photonic devices.

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Muons cosmiques au niveau de la mer

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Code : 463832 **Commission** :physique **Salle** :3

Mots clés : Muons, Flux et Simulation Monte, Carlo

Abstract :

Les rayons cosmiques (RCP) sont des particules neutres ou chargées qui proviennent de l'espace interstellaire et atteignent la Terre. À leur arrivée dans l'atmosphère terrestre, ces particules interagissent avec les atomes et les molécules, ce qui produit des particules secondaires. Les muons font partie de ces particules et constituent la composante dominante du rayonnement cosmique secondaire chargé qui atteint le sol. Nous présentons les mesures de la distributions des muons au niveau de la mer dans la direction nord-sud. La détection des muons a été effectuée avec deux détecteurs à scintillation NaI(Tl). Une épaisseur de plomb ajustable placée entre les détecteurs a permis de sélectionner des muons avec une impulsion minimale comprise entre 0,3 et 0,9 GeV/c. Le flux de muons intégré et différentiel a été déterminé en analysant les spectres d'énergie déposée dans les scintillateurs, soutenus par une simulation Geant4 [1, 2].

[1] I. Briki, M. Mazouz, and L. Ghedira, Measurement of the momentum dependence of atmospheric muon vertical intensity at ground level in Tunisia, Astroparticle Physics 134-135, 102657 (2022).

[2] Issa Briki and Malek Mazouz and Lotfi Ghedira, Angular distribution of low momentum atmospheric muons at ground level, Journal of Cosmology and Astroparticle Physics, (2023).

JDD2023 :8-9 Mai 2023

Approche quantique par l'algèbre de Lie pour les molécules diatomiques.

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Code : 468001 **Commission** :physique **Salle** :3

Mots clés : algèbre de Lie, interaction de type coulombienne, méthode ab, initio

Abstract :

Nous avons développé un modèle mathématique basé sur l'algèbre de Lie qui permet de traiter les interactions de type coulombienne. La validation du modèle passe par une comparaison avec les méthodes ab-initio classique de la chaine de Toulouse et avec des résultats expérimentaux pour le système étudié. La comparaison montre la fiabilité du modèle mathématique qui donne d'informations avec grande précision.

JDD2023 :8-9 Mai 2023

Electron and Phonon Tranports in a 3D FinFET Transistor

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Code : 468072 **Commission** :Electro **Salle** :3

Mots clés : BDE model, D, D model, FinFET, Self Heating Effect (SHE)

Abstract :

The switch from planar MOSFET to 3-D FinFET technology is one of the best choices to enhance electric performance, even though this switch could damage the transistor due to Self-Heating effect (SHE). In our wok, an electro-thermal model is developed by coupling the drift-diffusion model with the ballistic-diffusive-equation to evaluate the electrical and thermal characteristics of 14-nm Bulk and SOI FinFET devices. By giving comparisons of the I-V characteristics of our model with experimental data reported by INTEL and HP laboratories and numerical data given by TCAD simulators, the validity of the electrical part is verified. Thermal results are also improved by giving comparisons of our thermal characteristics with those obtained by TCAD simulators. The results analysis reveals that the temperature rises slowly in the case of Bulk FinFET comparing to SOI FinFET.

JDD2023 :8-9 Mai 2023

Investigation of the olfactory perception of odorants thiols on the human olfactory receptor OR2M3 via an advanced statistical physics modeling

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Code : 468453 **Commission** :chimie **Salle** :3

Mots clés : Statistical physics modeling, 3, mercapto, 2, methylbutan, 1, ol, 3, mercapto, 2, methylpentan, 1, ol, OR2M3, Receptor size distribution (RPSD), Adsorption energy distribution (AED)

Abstract :

In the present paper, a putative adsorption process of two odorants thiols (3-mercapto-2-methylbutan-1-ol and 3-mercapto-2-methylpentan-1-ol) on the human olfactory receptor OR2M3 has been investigated via advanced models developed by a grand canonical formalism of statistical physics. For the two olfactory systems, a monolayer model with two types of energy (ML2E) has been selected to correlate with the experimental data. The physicochemical analysis of the statistical physics modeling results showed that the adsorption system of the two odorants was multimolecular. Furthermore, the molar adsorption energies were inferior to 22.7 kJ/mol, which confirmed the physisorption process of the adsorption of the two odorant thiols on OR2M3. In addition, quantitative characterizations of both odorants were determined via the olfactory receptor pore size distribution (RPSD) and the adsorption energy distribution (AED), which were spread out from 0.25 to 1.25 nm and from 5 to 35 kJ/mol, respectively. For thermodynamic characterization of the olfactory process. Besides, the used model showed that the presence of copper ions increases the efficacy (olfactory response at saturation) of 3-mercapt-2-methylpentan-1-ol odorant activating OR2M3. The docking molecular simulation indicated that the 3-mercapto-2-methylpentan-1-ol molecule presented more binding affinities (17.15 kJ/mol) with olfactory receptor OR2M3 than 3-mercapto-2-methylbutan-1-ol (14.64 kJ/mol).

JDD2023 :8-9 Mai 2023

Structural, Mechanical and Electronic Proprieties of a Novel Braceletlike AsBiX3 (X = S, Se) Monolayers: A density functional study

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Code : 468861 **Commission** :physique **Salle** :3

Mots clés : First principles calculations, Auxetic materials, Mechanical stability, Semiconductors.

Abstract :

Through first-principles calculations, new ternary 2D auxetic materials, called AsBiX3 (X = S, Se) monolayers, have been predicted. These monolayers possess a unique bracelet-like configuration, resulting in a remarkably high in-plane negative Poisson's ratio (NPR) and a significant mechanical anisotropy. The thermal and mechanical stability of these monolayers has been confirmed by ab initio molecular dynamics simulations and elastic constant calculations, respectively. Our PBE calculations of the band gap have shown that these materials exhibit an indirect band gap semiconductor nature of 1.08 eV and 0.96 eV for AsBiS3 and AsBiSe3, respectively. When the spin-orbit coupling (SOC) is considered the band gap decreases by about 15 %. Furthermore, our study has identified that the p-As, p-Bi, and p-S/Se orbitals are mainly responsible for the conduction band minima, whereas the valence band maxima are dominated by the p-orbitals of chalcogen atoms, with a small contribution from the s-orbitals of As atoms. These findings demonstrate that AsBiX3 (X = S, Se) monolayers are promising candidates for applications in nanoelectronics and low-dimensional electromechanical devices.

JDD2023 :8-9 Mai 2023

Electrical polarization effects on the thermal response of FinFET nanotransistors

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Code : 468884 **Commission** :Electro **Salle** :3

Mots clés : FinFET transistor, numerical modeling, electrothermal modeling, short channel effect (SCE), ballistic diffusive effect (BDE).

Abstract :

FinFET is the nanoscale of MOSFET transistors. Due to miniaturization in MOSFETs, thermal effects have appeared. Particularly, phonon transport in semiconductor materials is a crucial problem. Additionally, this miniaturization includes several issues, such as short-channel effects. The challenge for FinFETs is to reduce these parasitic effects in order to increase the switching speed of a logic gate. In this paper, we propose a numerical investigation novel FinFET devices of a 20 nm and 10 nm. Numerical simulations, based on an electrothermal model, have been carried out using finite element method (FEM) integrated in COMSOL Multiphysics. We performed a comprehensive study of the gate length effects on the electrothermal response of FinFETs. Numerical simulations show that the power dissipation increases linearly with drain bias and achieved 1.12*10^15 and 6.2*10^15 W/m^3 for Lg=20 nm and Lg=10 nm, respectively. The remarkable difference of the Joule effect between Lg=20 nm and Lg=10 nm, can increase the device temperature when Lg decreases. In addition, the investigation of self-heating effect (SHE) is reported the critical temperature, which is responsible to vanish the drain current, is from 380 to 460 K for Lg = 20 and 10 nm, respectively.

JDD2023 :8-9 Mai 2023

study the mechanism of taste

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Code : 468937 **Commission** :physique **Salle** :3

Mots clés : Statistical physics model, Taste, Gerbil receptor site (GCaMP3), five principal tastes.

Abstract :

This study presents a contribution to the comprehension of the taste process at the molecular level, for the sweet taste at the level of the taste receptor sites.This investigation was established by using a putative adsorption process with involving a statistical model. This study makes a significant contribution to the comprehension of the tasting process of four molecules. It was possible to identify the number of adsorbed molecules per site (n), the density of receptor site (Nm), the half-saturation concentration (C1/2) and the molar energy of adsorption. The physico-chemical model parameters can be used for the energetic characterization of the interactions between the four entities and the rat taste receptor site, as well as for the determination of the taste band of the flavor, through the identification of adsorption energy values and adsorption energy distributions (AED).Also, a new investigation allows a determining of the taste band with the use of the best fitting model, and for describing the static and the dynamic sensitivities through the expression of the flavors response.

JDD2023 :8-9 Mai 2023

Electronic and nonlinear optical properties in spheroid-shaped core/shell quantum dot: effect of nanodot shape, eccentricity and dielectric environment

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Code : 469214 **Commission** :physique **Salle** :3

Mots clés : Spheroid core/shell quantum dots, Effective Mass Approximation, Nonlinear susceptibility, Dielectric matrix

Abstract :

In this work, we have performed a theoretical investigation of the electronic and nonlinear optical properties in prolate spheroid-shaped CdTe/ZnTe core/shell quantum dots (CSQDs) embedded in dielectric matrix (PVA, SiO2). The electronic band structure and the set of the wave functions were calculated by solving the Schrödinger equation within the framework of the Effective Mass Approximation (E.M.A) and taking in consideration the Compact Density Matrix (CDM). The dielectric mismatch effect between the system and the surrounding matrix is considered. Our numerical results revealed that the third-order nonlinear optical susceptibility is strongly influenced by the shape of QDs and the immersed dielectric medium (D.M). In addition, the suitable choice of the D.M with a higher dielectric constant (case of PVA) offers the possibility of tuning the nonlinear optical properties which are important for optoelectronic and photonic devices.

JDD2023 :8-9 Mai 2023

Stark shift of the intersubband transitions in Ge/Si1-xGex Step Quantum Well (SQW)

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Code : 469277 **Commission** :physique **Salle** :3

Mots clés : Step Quantum, Well, Intersubband transition, Optical absorption coefficient

Abstract :

In this work, we theoretically investigated of strained (Ge/Si0.03Ge0.97)/ Si0.15Ge0.85 Step Quantum Well (SQW) in the Terahertz (THz) region. The energy-level and the wavelengths of the intersubband transitions in the Ge/SiGe SQW are obtained by solving the one-dimensional Schrödinger equation. Then, the absorption spectra dependencies on the applied electric field from zero up to 50 kV/cm have been calculated at room temperature. A strong absorption coefficient (> 1×103 cm−1) and a Stark shift of the intersubband transition between 16 THz mm and 11 THz mm are demonstrated. The explored band structure parameters at strained Ge/SiGe SQW are useful tools for optoelectronic applications.

JDD2023 :8-9 Mai 2023

Non-relativistic ab initio investigation on the spectroscopic and radiative properties of the low lying electronic states of LiO and LiO+ molecules

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Code : 469312 **Commission** :physique **Salle** :3

Mots clés : Potential energy curves, Dipole moments, Radiative lifetimes, Einstein coefficients

Abstract :

Abstract: Exploring the properties of LiO and LiO+ could pave the way for advancements in energy storage, environmental remediation, chemical synthesis, making them promising candidates for developing novel technologies [1-2]. Thus, we present a non-relativistic ab initio investigation of LiO et LiO+ neutral and ionic molecules. The potential energy curves of the ground and low-lying excited states of LiO and LiO+ are calculated at the MRCI+Q level of theory associated with the aug-cc-pV5Z basis sets. Several properties such as the equilibrium distances, dissociation energies, harmonic and anharmonic frequencies, rotational constants, permanent and transition dipole moments, vibrational energies, Franck-Condon factors, and radiative lifetimes including bound-bound and bound-free transitions are predicted. The data obtained will be useful for further experimental and theoretical studies. References: [1] M. Yoshimine, Accurate potential curves and properties for the X2Π and A2Σ+ states of LiO, J. Chem. Phys. 57 (1972) 1108–1115. [2]Da Silva, R. S., & Ballester, M. Y. (2021). Theoretical study of the low-lying doublet and quartet electronic states of 7Li16O molecule including spin-orbit coupling effect and a new limit to the adiabatic ionization energy. Chemical Physics, 545, 111123.

JDD2023 :8-9 Mai 2023

FPGA implementation of neural network for classification of nervous system and brain diseases.

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Code : 469390 **Commission** :Electro **Salle** :3

Mots clés : Neural network, neuron, dendrite, chaotic, EEG, ECG

Abstract :

The human brain is a complex network of neurons. It is known that the human brain has 1010 neurons. Each neuron controls and drives the dynamical behaviour of organs. Recently, researchers have been exploring the application of machine learning models to connectome data in order to predict clinical outcomes and analyse the importance of sub networks in the brain. Connectome data has unique properties, which present both special challenges and opportunities when used for machine learning . After decades, many artificial neural networks have been proposed to develop tools that may lead to a better understanding of the behavior of brain. Their various versions have also been intensively and extensively studied in many aspects and successfully applied to many fields such as identifying pattern, recognizing voice, controlling system, processing signal systems, treating static image, and solving nonlinear algebraic system. In this thesis, we look for generation a new tools based on neural networks to classify brain disorder such as: - Autism, - Alzheimer, - Schizophrenia.

JDD2023 :8-9 Mai 2023

Efficient Architecture based AES cryptographic algorithm

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Code : 469580 **Commission** :Electro **Salle** :3

Mots clés : cryptography, memristor, AES

Abstract :

Due to technological developments of the Internet of Things, the use of electronic devices has become more useful for sharing information. Data security is an important constraint in protecting confidential information. This paper proposes a new innovative solution to improve the advanced encryption standard (AES) efficiency, speed, and power consumption. Memristor design is used to achieve goals and solve CMOS limitations.