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Optical & Electrical Properties of BOROPHENE from the BRUS Model and Characteristic Matrix Theory

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Abstract

In this paper, we studied the physical properties (optical and electrical) ofboropheneas a function of change in size using the MATLAB program.To compute these properties as a function of change in the nanoparticlesize, we relied on the Brus model and the characteristic matrix theory as atheoretical basis.

Keyword: Borophene,BruceModel,Matrix,materialsandopticalproperties.

1. Introduction

The first two-dimensional material to be discovered was graphene [1]. Asmany of the amazing properties of graphene were investigated, a series ofnewmaterialsknownas"2Dmaterials"[2]werediscovered.2Dmaterials are still relatively new, and becoming an exciting field of manyapplications[3].Typically,two-dimensionalmaterialshaveseveraldistinctphysicalpropertiesthatarepromisingforelectronicdevices,nanoscale engineering, energy conversion, and photonics [4]. With therapiddevelopmentofgrapheme,other2Dmaterials,suchasphosphorene,BN,germanene,antimonene,silicene,arsenene,andtransition metal dichalcogenides, have recently arisen extensive interest, agroupofmaterialswithatomicthicknessesthataretheoreticallypredicted orsynthesized[5]havebeenproposed.Amongtheseproposedmaterials is Borophene, a monolayer of crystallized boron, also known as a boronpaper. It was first predicted theoretically in the mid-1990s, [6] and in2015,a2Dboronmonolayerwassuccessfullysynthesizedonsilver(Ag) [7]substrates.

The study of borophene has attracted many researchers from many fields,such as material science, nanotechnology, physics, and chemistry [8]. It isalso considered the lightest two-dimensional material to date. Boropheneis a neighbor of graphene, and hence, some similar properties to grapheneareexpected[9].

The mechanical properties ofBorophene are particularly interesting andimportant. First, Borophene has a low surfacemass density. with a hightensilestrength&intoplanestiffness,borophenecanbeusedasanau

xiliaryfordesigningcompounds.Second,withahighflexibilityboroph eneisalsosuitableforthefabricationofflexiblenanoscaledevices[10]. Moreover, due to the strongly varyingstructural propertiesof borophene , including its magnetic and electronic properties, it can beeffectively controlled for multiple applications [11]. Since boron atomsarerichinbondingconfigurations,boropheneispolymorphic,wh ichincreases its differentiation from other two-dimensional materials [12]. Inshort, borophene is rich in resources, has low atomic mass (light weight),lowcostandhasexcellentelectricalproperties.Theseadvantag esofBoropheneprovidemanypossibilitiesforpracticalapplicationinth efuture.

2. Theory:

A. Brus model:

The first theoretical calculation of nanostructured semiconductor particlesbased on effective mass approximation (EMA) is reported by Brus[13].Inthisapproximation,theexcitonisconsideredtobeconfinedt oasphericalvolumeofthecrystalandthemassesofelectronsandholesar e replacedbyeffectivemasses($m^*$and m^*)todeterminetheenergy gap:

Where $r_{ps}$is the radius of the particle, $m^*$is the effective mass of thehole,m^*istheeffectivemassoftheelectronandεistherelativepermittivity, or what is known as the dielectric constant. The energy gapthenis[14]:gap in quantum dots. In the first term of equation (1) we can observe thatthe energy gap is inversely proportional to r^2as the energy gap increasesas the particle size decreases. In the second equation, we can observe thatthe energy gap decreases with decreasing r_{ps} as a result of increasing thestrength of the coulombic interaction. The second and third terms are verysmall compared to the first, so they can be neglected. Next, equation (2)becomes:we would expect the energy gap to increase with decreasing particle sizedue to the effect of quantum confinement, which has a large effect whentheparticleradiusr_{ps}isequaltoorsmallerthantheBohrradiusfor Excitonα∘[15]:

Where $\varepsilon_r$and $\varepsilon_\circ$are the permittivities of the semiconductor and of thevacuum,respectively.

B. Relationshipbetweenenergygapandrefractiveindex:

There is a close correlation between the energy gap $E_g$and the refractiveindex n, and many studies have been conducted to find mathematicalformulaslinkingtherefractiveindexwiththeenergygapa ndthefollowingrelationship isthemost commonlyaccepted [16]:

Given the simple physics of light refraction and scattering, an empiricalrelationshiphasbeenproposed.

In equation(5) , since β<0, we see that the refractive index

decreaseswhen the energy gap increases. From equation (3), we can say that therefractiveindex ofquantumdots decreases astheparticlesizedecreases.

C. Thecharacteristicmatrixofasinglethinfilm:

Thecharacteristicmatrixlinkingthetangentialcomponentsoftheelectri cand magneticfields can beexpressed as follows [17]SinceReistherealpartofthequantity(5_{sub}).

3. application

A. Thestudyof opticalproperties:

The energy gap of Borophene was studied as a function of the size of theparticle Ps, which is given to the quantum points through the followingrelationship:$Ps = 2r_{ps}$(r_{ps}representstheradiusoftheparticlesofmatter) [22]. The material particle size values were chosen ranging from6nm to 40nm . Most semiconducting materials behave visually similarlywhen the particle size of the material decreases from the bulk size, as aresult of volume quantization .This behavior arises because the size of thenanoparticles is comparable to the De Broglie wavelength of their chargecarriers (i.e. electronsandholes). We notice inthe figure(1) thatthevalue of the energy gap is large at small volumes and then graduallydecreases when the size of the object increases until it becomes almostconstant after the particle size of the material exceeds for rad radius bohrforexcitonradiusofmostmaterials,[23].

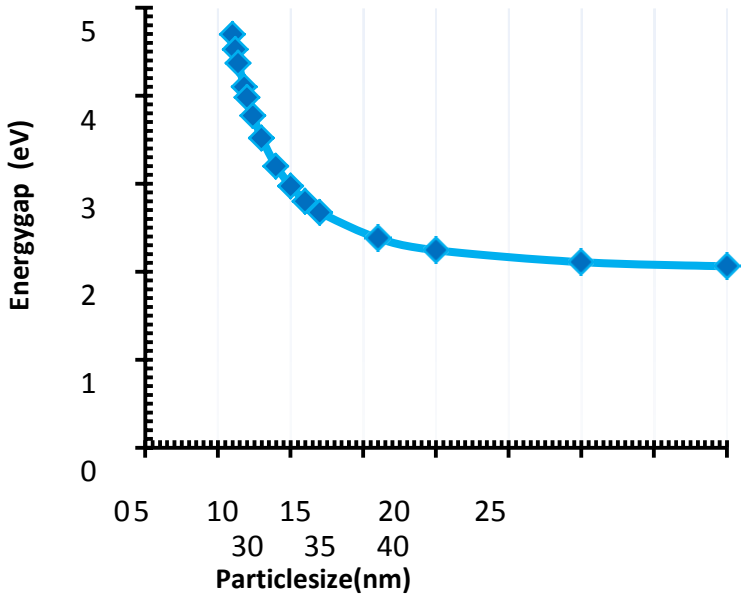

figure (1): Energy gap change for BoropheneAs a function of the changeinthe nanoparticle size.

From studying the refractive index, we find that it becomes almostconstantfornanoscalesizes(30-

40nm)andgreaterthanthat,asduetothefact that the material in this case behaves its behavior in its normal state(Bulk material), the material can be considered the material is isotropic,but with a decrease in the particle size of the material less than (30 nm).The refractive index begins to decrease gradually and thus there is adirectrelationshipbetweenitandthevolume,andthisdecreaseisduetot he quantitative confinement and to explain this, the effects of quantumseizure begin roughly when the particle diameter is reduced to a valueequal to or smaller than the exciton diameter of Bohr, which led to thephenomenon of electron confinement and a gradual increase in theexcitonic transition energy (band gap) with a decrease in the mass size[24].

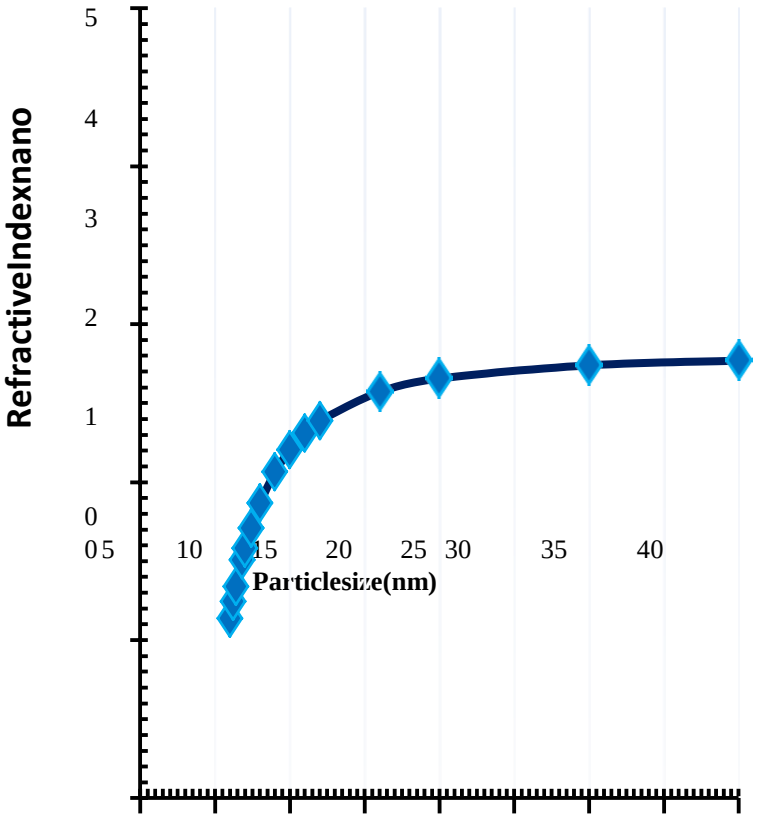

figure (2): Refractive index change for BoropheneAs a function of thechangeinthe nanoparticlesize.

And when we study the reflectivity, we notice from figure (3) that whenthe granular size is small or when the granular size decreases, then theborophenetendstobepermeabletoelectromagneticradiation.Forlo ngergranularsizesandthereflectivityconvergetothebulkvalueboroph ene tends to be reflective (R = 52%) Absorbance is neglected andtheequationisinterpreted:

T+R +A=1withA=0[25]

This study is an approximation of what was found by Zhi-Qiang Wangand others[5].

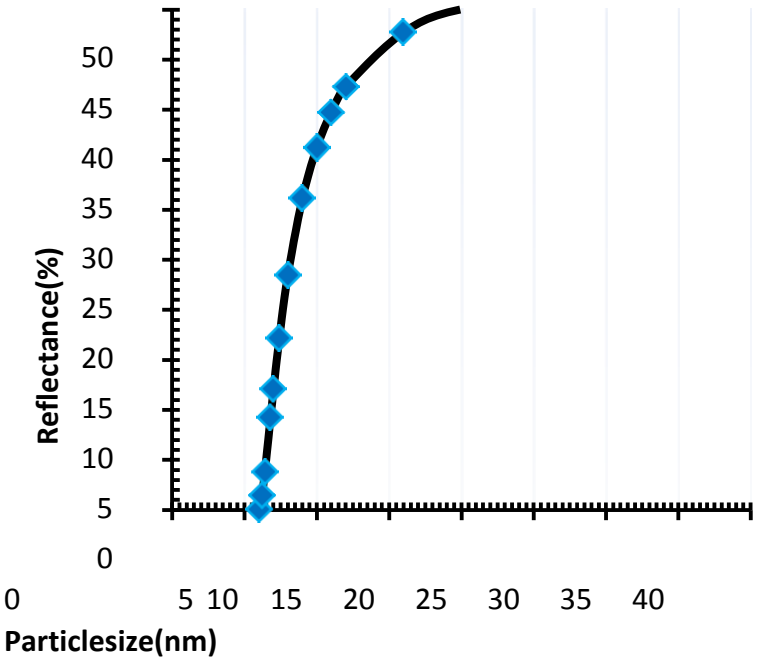

figure (3): Reflectivity change for BoropheneAs a function of the changeinthe nanoparticle size.

B. Studyofelectrical properties:

When studying the dielectric constant of Borophene, we notice that thedielectric constant decreases with the nanoscale (figure(4)). this can beunderstoodbynotingthatforsmallparticlesizes,thenumberofsurfaceatoms is relatively large . But for nanomaterials, the number of atoms perunit volume will decrease due to quantitative confinement. Where in thenanoscale scale, the electron orbits around the nodes causing an increasein the coulomb force which promotes the force recovery. Hence, thenatural angular frequency of the electron oscillation, which causes thedielectric constant to decrease, and this proves that the dielectric constantdecreases withtheparticlesize ofthe material[26].

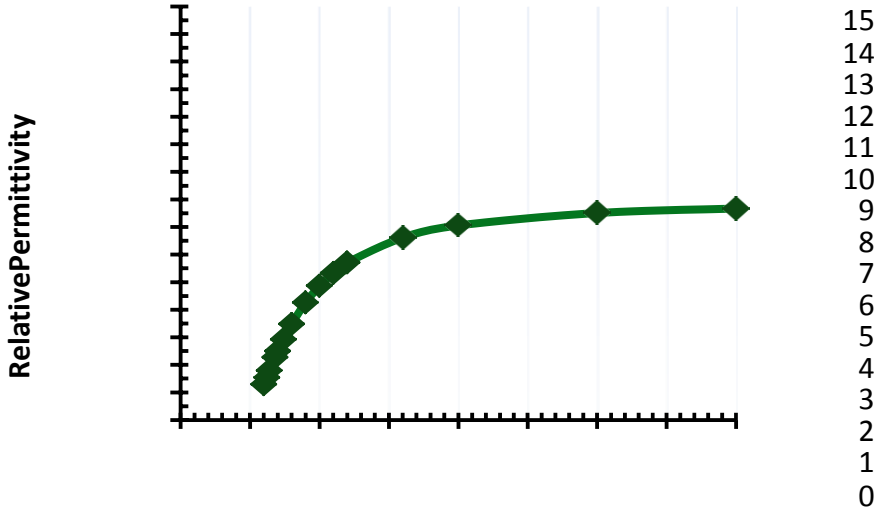

figure (4): Dielectric constant change for BoropheneAs a function of thechangeinthe nanoparticlesize.

When studying the activation energy, we notice that the valuesare largeat small nanoscale sizes, and decrease as the body size increases andapproachestheBohrradiusoftheexciton.Whencomparingtheactivation energy curve with the energy gap curve figure (5) , we notice agreat similarity . This is due to the activation energy is across the Fermilevel,whichislocatedintheenergygap.thisimpliesthattheactivation

energyisequaltohalftheenergygap[27],andthechangeintheactivation energy is directly proportional to the change in the energy gap,figure(5) .

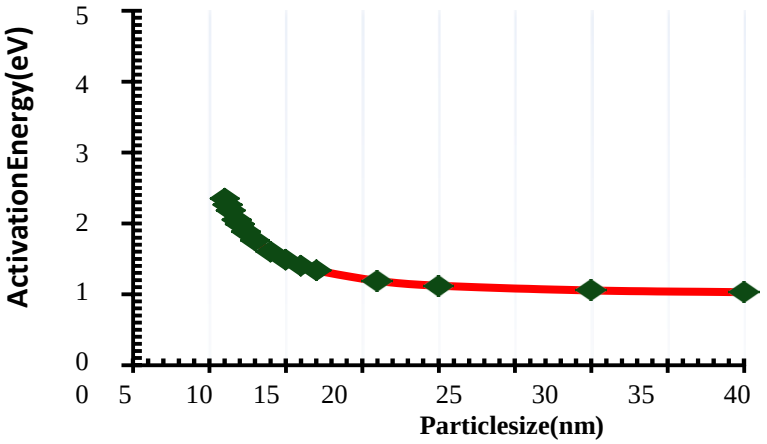

figure (5): Activation energy change for BoropheneAs a function of thechangeinthe nanoparticlesize.

When studying the concentration of charge carriers, we notice when thesize is very small, the concentration of charge carriers is very small .Thisis due to the quantitative confinement to the electron for the small sizes,where the atoms present on the surface are few. The particle size of thebody increased, the greater the number of atoms and molecules on thesurface, in other words, the increase in charge carriers (electrons andholes) in the semiconductors, and thus the conductivity of the materialsincreased accordingtotheincrease ofthesecarriers.

This behavior was observed by P. Parameshwari (2012), who emphasizedthattheincreaseinelectricalconductivitycanbeattributedtothedecreaseindispersionthatoccursattheboundariesofthegrainswhen

increasingthesizeofthegranules,whichleadstoanincreaseinthemobilityand injectionoffreechargecarriers[28].In thefigurebelow.

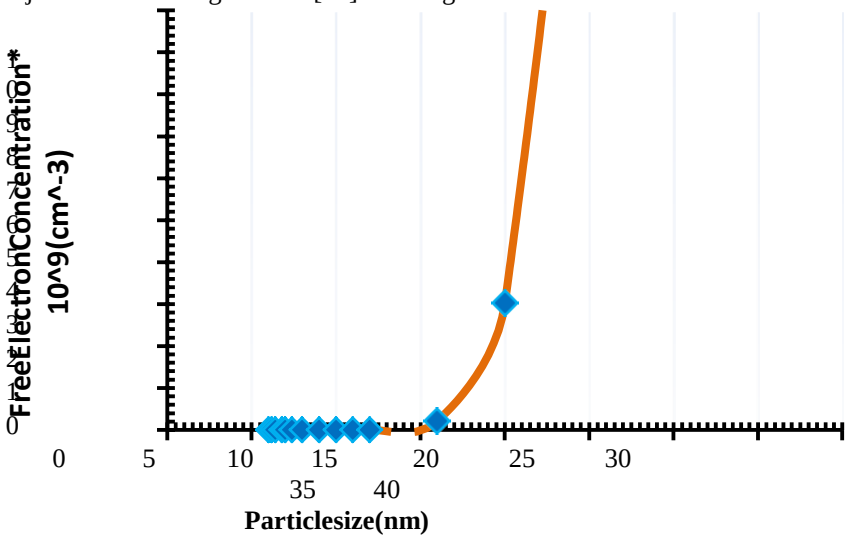

figure (6): Concentration of charge carriers change for BoropheneAs afunctionofthechange inthenanoparticlesize.

Conclusion:

We noticed that there is a significant correlation between the physicalproperties (optical and electrical) of Borophene and the particle size, aswhen the particle radius of the material is equal to or smaller than thebohr radius of the Exciton, the refractive index will decrease and theenergy gap increases with the decrease in the particle size, and this leadsto a decrease The reflectivity of materials with reduced particle size, duetothe effectof quantumconfinement.

We also note that whenever the size of the particle decreases, thedielectric constant will decrease and the activation energy will increase.Also, when the volume is very small, the concentration of the chargecarriers is very small and this is due to the quantitative confinement of theelectron for thesmallsizes.

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