COMPUTATIONAL MODELLING OF LIGHT-MATTER INTERACTION IN AMORPHOUS SILICON WITH QUANTUM DOT FOR SOLAR CELL APPLICATIONS

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“Not everything is as simple as Simple Harmonic Motion.” – Mirzaldehyde (2015)

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We are like intertwined stars in the vast galaxy.

ABSTRACT

As the world population rises, energy needs, including power generation, are becoming critical; using photovoltaic technologies like amorphous silicon solar cells (aSiSC) to harness solar energy might benefit global concerns. Recent investigations stated that aSiSCs were poor short-wavelength absorbers. Quantum dot (QD) technology may be applied to aSiSC to improve optical absorptions and electric fields since the QDs' bandgap is tunable, spanning a larger electromagnetic spectrum. However, the computational approach to QD properties is not yet computationally summarised. Here, this work focuses on the fundamental design of a 3D quantum dots amorphous silicon solar cell (aSiQDSC) model with various core sizes of core/shell QD to identify the optical absorption peak, electric field profiles, and light-matter interaction process. This study used COMSOL Multiphysics software to simulate utilising the finite element model (FEM). The aSiSC model's optical absorption peaked at 736 nm at 41.83%. For aSiQDSC models, type-I QD: cadmium selenide/zinc sulphide (CdSe/ZnS) with 0.5 nm core radius produced the maximum optical absorption, 46.01% at 642 nm, compared to type-II: cadmium telluride/cadmium selenide (CdTe/CdSe) and inverted-type-I: cadmium telluride/indium phosphide (CdTe/InP). As the QD core radius diminished, optical absorption peaks and electric fields rose. The quantum confinement effect (QCE) causes multi-exciton generations (MEG) within the QD to provide advantages to aSi. This study continued by combining nanocavity (NC) and nanoantenna (NA) to increase optical absorption and electric fields. In the presence of gold (Au) rectangular (5×5×3) nm nanosheets NA, the model showed higher optical absorption of 46.58% at 642 nm due to strongly restrained electric fields, creating a hot spot in the 0.5 nm nanogap resulting in localised surface plasmon resonance (LPSR). Ultimately, the largest cavity aperture hemi-ellipsoidal NC with 8.0 nm in the aSiQDNANCSC model amplified the optical absorption with 47.00% at 641 nm. Computationally, this model design is an environment-friendly, high-absorption, and electric fields SC that will enable future research and fabrication.

ABSTRAK

Peningkatan populasi dunia dan keperluan sumber tenaga seperti penjanaan kuasa adalah semakin genting. Teknologi fotovoltan seperti sel suria silikon amorf (aSiSC) untuk menyerap tenaga solar adalah bermanfaat kepada sejagat. aSiSC diwartakan penyerap panjang gelombang pendek yang lemah. Teknologi bintik kuantum (QD) boleh diterapkan ke dalam aSiSC untuk meningkatkan penyerapan optik dan medan elektrik atas jurang jalurnya yang boleh ditala, merentangi spektrum elektromagnet yang luas. Namun, pendekatan pengiraan ciri-ciri QD masih belum disimpulkan. Oleh itu, penyelidikan ini fokus kepada asas rekabentuk 3D sel suria QD silikon amorf (aSiQDSC) dengan beberapa saiz teras bagi QD teras/petala untuk mengkaji puncak serapan optik, medan elektrik, dan proses interaksi cahaya dan jirim. Kajian ini menggunakan perisian COMSOL Multiphysics dengan menggunakan model unsur terhingga (FEM). Puncak penyerapan optik bagi aSiSC adalah pada 736 nm sebanyak 41.83%. Bagi model aSiQDSC, QD jenis-I: CdSe/ZnS dengan jejari teras 0.5 nm menghasilkan penyerapan optik yang tinggi, 46.01% pada 642 nm, berbanding dengan jenis-II: CdTe/CdSe dan songsangan-jenis-I: CdTe/InP. Apabila jejari teras QD mengecil, puncak penyerapan optik dan medan elektrik meningkat. Kesan pengurungan kuantum (QCE) menyebabkan berlakunya penghasilan berbilang eksiton (MEG) dalam QD, manfaat kepada aSi. Kajian ini diteruskan dengan menggabungkan ruangannano (NC) dan antenanano (NA) untuk meningkatkan penyerapan optik dan medan elektrik. Penggunaan kepingannano emas (Au) segi empat (5×5×3) nm NA, model menunjukkan penyerapan optik, 46.58% pada 642 nm disebabkan oleh medan elektrik yang dikawal kuat menghasilkan titik panas pada 0.5 nm ruangnano yang mengakibatkan resonans permukaan plasmon setempat (LSPR). Bagi reka bentuk terakhir, aSiQDNANCSC, ruangan bukaan terbesar NC hemielipsoid, 8.0 nm menggandakan penyerapan optik, 47.00% pada 641 nm. Khususnya, model ini adalah mesra alam, sel suria dengan penyerapan optik dan medan elektrik yang tinggi membuka ruang kepada penyelidikan dan penghasilan pada masa akan datang.

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LIST OF SYMBOLS AND ABBREVIATIONS

a	–	Nanocavity aperture
A	–	Absorption
A_p	–	Absorption peak
B	–	Magnetic flux density
c	–	Speed of light
cm^{-3}	–	Per centimetre cube
C_n	–	Electron capture cross section constant
C_p	–	Hole capture cross section constant
D	–	Electric flux density
d	–	Differential operator
D_n	–	Electron electric flux density
D_p	–	Hole electric flux density
E	–	Electric field intensity
e	–	Electron charge
E_c	–	Conduction energy band
E_g	–	Energy bandgap
E_{gc}	–	Core energy bandgap
E_{gs}	–	Shell energy bandgap
E_m	–	Maximum electric field intensity
E_n	–	n^{th} energy level
E_n	–	Electron energy state
E_t	–	Energy trap state
E_v	–	Valence energy band
f_0	–	Particle natural frequency
f_F	–	Probability function of Fermi-Dirac statistics

FF	–	Fill factor
f_{F0}	–	Probability function at thermal equilibrium
g	–	Nanogap of nanoantenna
g_c	–	Quantum state density in the conduction band
g_v	–	Quantum state density in the valence band
$\mathbf{H}$	–	Magnetic field intensity
h	–	Planck constant
$\hbar$	–	Reduced Planck's constant
i	–	Imaginary part
I	–	Electromagnetic wave intensity
I_0	–	Incident electromagnetic wave intensity
$\mathbf{J}$	–	Current density
J_{sc}	–	Short-circuit current
k_B	–	Boltzmann's constant
k_n	–	Wave number
k_r	–	Extinction coefficient/refractive index (imaginary)
L	–	Size of potential well
l	–	Length of model
log	–	Logarithmic function
L_x	–	Potential well length for *x*-axis
L_y	–	Potential well length for *y*-axis
L_z	–	Potential well length for *z*-axis
m	–	Mass
m^*	–	Effective mass
m_0	–	Effective mass
m_e	–	Electron mass
m_h	–	Hole mass
n	–	Electron distribution concentration
$\mathbf{n}$	–	Normal vector
n'	–	Electron concentration at the trap energy state
n_0	–	Electron concentration at thermal equilibrium

n_1	–	Refractive index of the first medium
n_2	–	Refractive index of the second medium
N_c	–	Electron effective density of state
n_i	–	Intrinsic semiconductor
n_r	–	Refractive index (real)
N_t	–	Total concentration of the trapping centre
n^{th}	–	Number
Nv	–	Hole effective density of state
o	–	o-semiaxis of nanocavity
p	–	Hole distribution concentration
P	–	Electrical power
p'	–	Hole concentration at the trap energy state
p-	–	Scattering p-parameter
P_{i1}	–	Incident electromagnetic wave power on port one
P_{i2}	–	Incident electromagnetic wave power on port two
P_{r1}	–	Reflected electromagnetic wave power on port one
q	–	q-semiaxis of nanocavity
R	–	Reflection
r_b	–	Exciton Bohr's radius
r_c	–	Core radius
R_{cn}	–	Electron capture rate
R_{en}	–	Electron return rate
R_n	–	Electron recombination rate
R_p	–	Reflectance of transverse magnetic wave propagation
R_p	–	Hole recombination rate
r_s	–	Shell radius
R_s	–	Reflectance of transverse electric wave propagation
S	–	Surface area of nanoantenna
s-	–	Scattering s-parameter
s_{11}	–	Reflection scattering parameter
s_{21}	–	Transmission scattering parameter

S_a	–	Small surface area of nanoantenna
t	–	Time
t	–	Thickness of nanoantenna
T	–	Transmission
T	–	Absolute temperature
T_p	–	Transmittance of transverse magnetic wave propagation
T_s	–	Transmittance of transverse electric wave propagation
u	–	u-semiaxis of nanocavity
v	–	Particle velocity
V m^{-1}	–	Volt per metre
$V(x)$	–	Potential energy
V_{oc}	–	Open-circuit voltage
w	–	Width of model
x	–	Position
ε	–	Permittivity
ε_r	–	Relative permittivity/dielectric constant
η	–	Power conversion efficiency
θ_i	–	Incident electromagnetic wave angle
θ_t	–	Transmitted electromagnetic wave angle
λ	–	Wavelength
λ_p	–	Wavelength peak
μ	–	Permeability
μ^*	–	Charge carrier mobility
μ_e	–	Electron mobility
μ_h	–	Hole mobility
μ_n	–	Electron mobility
μ_p	–	Hole mobility
μ_r	–	Relative permeability
π	–	Constant number, pi = 3.14..
ρ	–	Charge density
σ	–	Conductivity

τ	–	Carrier's lifetime
τ_m	–	Particle lifetime
τ_n	–	Electron lifetime
τ_p	–	Hole lifetime
χ_0	–	Electron affinity
ψ	–	Wavefunction
ψ_e	–	Electron wavefunction/concentration
ψ_h	–	Hole wavefunction/concentration
∇	–	Del operator
$\bullet$	–	Dot product
$\times$	–	Cross product
%	–	Percentage
∂	–	Partial differential
ω	–	Angular frequency
1D	–	1-dimension
2D	–	2-dimension
3D	–	3-dimension
AFORS-HET	–	Automat for simulation of heterostructures
Ag	–	Silver
Al	–	Aluminium
AlAs	–	Aluminium arsenide
ANSYS	–	Analysis of system software
aSi	–	Amorphous silicon
aSiQDNANCSC	–	Amorphous silicon quantum dot nanoantenna nanocavity solar cell
aSiQDNASC	–	Amorphous silicon quantum dot nanoantenna solar cell
aSiQDSC	–	Amorphous silicon quantum dot solar cell
aSiSC	–	Amorphous silicon solar cell
Au	–	Gold
CB	–	Conduction band
CdS	–	Cadmium sulphide

CdSe	–	Cadmium selenide
CdTe	–	Cadmium telluride
CM	–	Carrier multiplication
COMSOL	–	Simulation software/tool
CPU	–	Central processing unit
cSi	–	Crystalline silicon
CTe	–	Carbon telluride
Cu	–	Copper
DoS	–	Density of states
EM	–	Electromagnetic
EMW	–	Electromagnetic wave
EQE	–	External quantum efficiency
eV	–	Electron volt
ewfd	–	Electromagnetic wave frequency domain
ewfd.Atotal	–	Total absorbance
ewfd.normE	–	Normalise electric field intensity expression
FDM	–	Finite difference method
FDTD	–	Finite-difference time-domain
FEA	–	Finite element analysis
FEM	–	Finite element method
GaAs	–	Gallium arsenide
GaN	–	Gallium nitride
Ge	–	Germanium
GeSi	–	Germanium-silicon
GPVDM	–	Organic photovoltaic device model software
HgS	–	Mercury sulphide
i-	–	Intrinsic semiconductor
InAs	–	Indium arsenide
InP	–	Indium phosphide
IR	–	Infrared
ITO	–	Indium tin oxide

LSP	–	Localised surface plasmon
LSPR	–	Localised surface plasmon resonance
MD	–	Molecular dynamic
MEG	–	Multi-exciton generations
MUMPS	–	Multifrontal massively parallel sparse direct solver
n-	–	Negative doped semiconductor
NA	–	Nanoantenna
NC	–	Nanocavity
nm	–	Nanometre
p-	–	Positive doped semiconductor
PBC	–	Periodic boundary condition
PbS	–	Lead(II) sulphide
PbSe	–	Lead selenide
PbTe	–	Lead telluride
PC	–	Personal computer
PC1D	–	One-dimensional device simulator
PC3D	–	Three-dimensional device simulator
PCE	–	Power conversion efficiency
PEC	–	Perfect electric conductor
PEDOT:PSS	–	Poly(3,4-ethylenedioxythiophene) polystyrene sulphonate
PL	–	Photoluminescence
PMC	–	Perfect magnetic conductor
PV	–	Photovoltaic
QCE	–	Quantum confinement effect
QD	–	Quantum dot
QDSC	–	Quantum dot solar cell
QED	–	Quantum electrodynamics
QY	–	Quantum yield
RAM	–	Random access memory
RF	–	Radio frequency
SC	–	Solar cell

semi.Ec	–	Conduction energy band expression
semi.Ev	–	Valence energy band expression
semi.N	–	Concentration of electron expression
semi.P	–	Concentration of hole expression
Si	–	Silicon
SiGeSn	–	Silicon-germanium-tin
SiO_2	–	Silicon dioxide
SnAgCu	–	Tin-silver-copper
SPP	–	Surface plasmon polariton
TCAD	–	Technology computer aided design
TE	–	Transverse electric
TM	–	Transverse magnetic
UV	–	Ultraviolet
VB	–	Valence band
VR	–	Visible region
ZnO	–	Zinc oxide
ZnS	–	Zinc sulphide
ZnSe	–	Zinc selenide

LIST OF PUBLICATIONS

1. Rodhuan, M. B., Abdul-Kahar, R., Ameruddin, A. S., Rus, A. Z. M., & Tay, K. G. (2023). Computational modelling of light-matter interaction in aSi with CdSe/ZnS core/shell quantum dots and metal nanoantenna for solar cell applications. *Physica Scripta*, *98*(5), 055012.
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4. Nasar, M. N., Abdul-Kahar, R., Amir Hamzah, N. S., Esa, F., & Rodhuan, M. B. (2019). Effect in Positioning Gold Nanoparticle inside Plasmonic Solar Cell on Absorption, Reflection and Transmission. *Universal Journal of Electrical and Electronic Engineering*, *6*(5B), 7-12.

CHAPTER 1

INTRODUCTION

1.1 Background of the study

As the global population grows and energy is in demand, the challenges of fossil energy exhaustion, greenhouse effect, and environmental issues become critical (Lu *et al.*, 2020; Channa *et al.*, 2020; Selopal, 2020; Ojo *et al.*, 2019). According to British Petroleum's yearly report in 2017 (Ojo *et al.*, 2019), the world depends on fossil fuels as primary sources of energy (Selopal, 2020; Abdulkarim *et al.*, 2019). It is almost 85% of total energy usage, 5% nuclear power, and 10% renewable energy resources—consequently, this movement is not sustainable and lead to catastrophic effect. Furthermore, renewable energy sources are replenishable over a human lifetime (Ojo *et al.*, 2019). Consequently, numerous efforts by the scientific team are devoted to replacing fossil fuels with renewable resources such as hydroelectric, biofuels, wind power, and solar energy (Selopal, 2020; Ahmad *et al.*, 2018; Wu *et al.*, 2016).

One of the most promising solutions to the global energy dilemma has been harnessing solar energy to generate electricity (Lee & Ebong, 2017). Solar energy is a readily available, unlimited, and environmentally benign energy source that meets the energy demands (Selopal, 2020; Abdulkarim *et al.*, 2019; Wu *et al.*, 2016), providing a chance to solve the energy crisis and reduce the environmental issues of the fossil fuel usage (Liu *et al.*, 2020). The sun's continual thermonuclear fusion generates energy, emits substantial electromagnetic radiation, and reaches Earth's surface with plentiful energy in an hour more than the world's annual energy consumption; this suggests that solar energy conversion is viable for meeting future energy requirements (Channa *et al.*, 2020; Ojo *et al.*, 2019).

The technology of solar power has advanced in focusing on larger areas, particularly photovoltaic (PV) technology, which captures energy from the ultraviolet (UV), visible light, and infrared spectrum (IR). The energy conversion of solar power into electricity focuses on PV energy conversion technology. The light-matter interaction process (Felicetti, 2015) converts solar power's exciting electrons into a direct current to generate electricity (Ojo *et al.*, 2019). The excited electrons in the PV device jump to a higher energy level by photons from the sunlight, permitting them to operate as charge carriers. The method warrants the utilisation of PV semiconductor materials, producing a depletion area where the electron-hole pairs are generated when high-energy photons with more significant energy than the material bandgap are injected, causing the charge carriers effectively separate before recombination occurs, and charge carrier conveyance over an external circuit (Ojo *et al.*, 2019; Bisquert, 2017). However, the solar cells' absorber could absorb light in a specified portion of the electromagnetic spectrum, representing that few lights were not absorbed while others transformed into heat (Ali *et al.*, 2018; Jasim, 2015).

Numerous solar technologies, specifically thin film, have been studied with tremendous results to attain dependability, cost-effectiveness, and high performance of devices (Lee & Ebong, 2017). Thin film technology is one most promising development in photovoltaic research (Jabeen & Haxha, 2018) where it has become the most demanding in commercialisation and rigorous development research as the size of thin films down to two microscales or less have effective absorption and flexibility (Jabeen & Haxha, 2019). According to Ojo *et al.* (2019), the material used as the absorber in manufacturing PV technology is classified as first-, second-, and third-generation solar cells. Solar cells (SC) based on silicon material (Si) comprise the first generation. First-generation SCs are the most firm of all SC types and are notable for their extensive use of bulk materials and high production costs. Second-generation SCs apply thin-film technology to minimise material fabrications and production costs. Third-generation SCs portray thinner films, lower fabrication temperatures, higher efficiency, and cheaper costs.

In a brief theoretical approach, the electromagnetic field (photon) interacts with matter in the solid state, the most fundamental physical process in solar cells, called the light-matter interaction process (Felicetti, 2015). The term 'light-matter interaction' covers classical theory to the quantum electrodynamics (QED) theory. The separation of light and matter topics occurred a long time ago and then reunited even more details as the increment of quantum mechanics changed people's perception of the behaviour of wave-particle duality to light and matter (Weiner & Nunes, 2017; Felicetti, 2015), as shown in Figure 1.1. Felicetti (2015) also explained that the light-matter interaction concept has a more comprehensive meaning, the interaction between bosonic fields (light) and anharmonic systems (matter), which effectively involves few energy levels. The 'interaction' terms showed that light and matter are different identities that influence one another by a mediator (Weiner & Nunes, 2017).

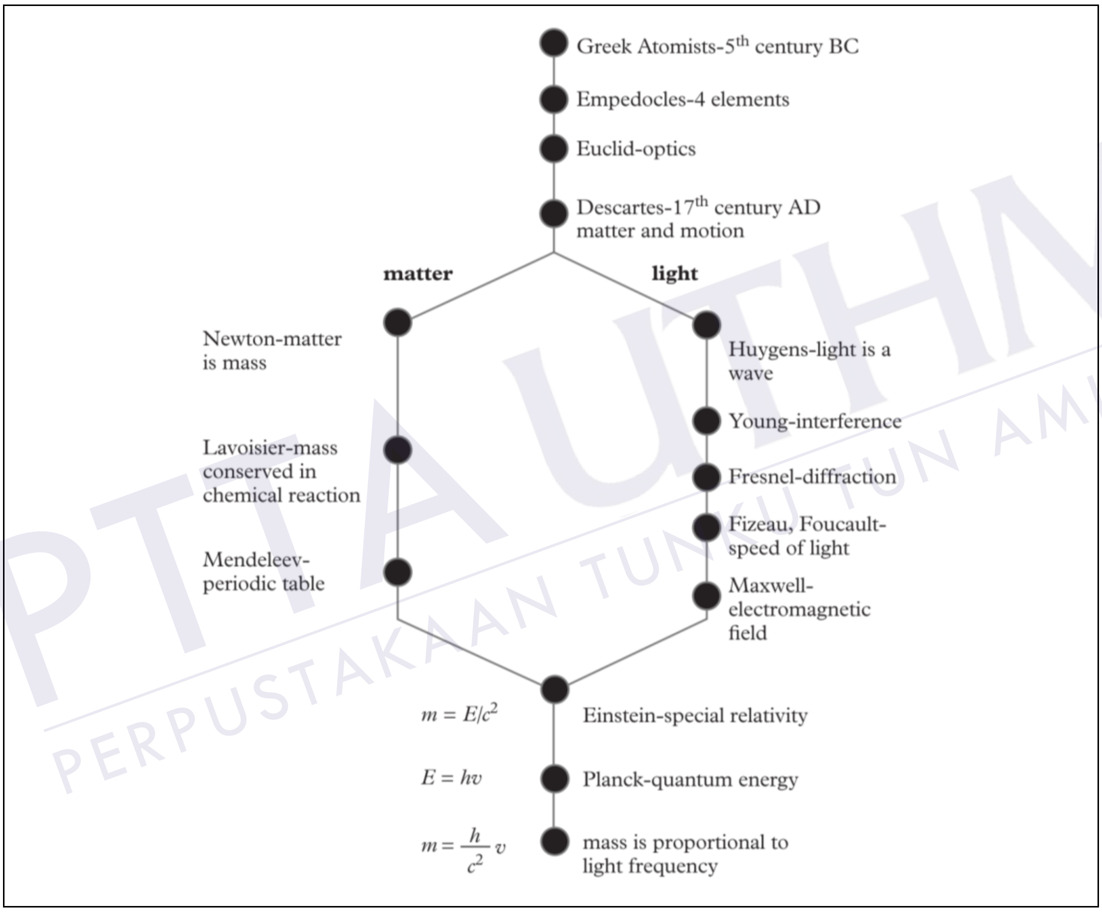

Figure 1.1: The brief history of light and matter interaction (Weiner & Nunes, 2017)

The unification of quantum applications and condensed matter physics culminated in the participation of the quantum dot (QD), a nanoparticle interconnected to light and matter (Tighineanu, 2015). The QD was declared an artificial atom since its crystalline structure and semiconductor behaviours are analogous to atomic structure and optical characteristics (Delgado *et al.*, 2020; Nideep *et al.*, 2019; Kantner, 2018; Slamet & Sahni, 2017; Schütz, 2015). Compared to the atomic

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VITA

The author birthed on November 29, 1995, in Kuantan, Pahang, Malaysia. He patronised his secondary school at SMK Sungai Isap, near his hometown. His study continued at Pahang Matriculation College (KMPh) in the same city in 2013. He contributed three modules of terminology, formula, and short notes, especially for students who enrolled in a Physics course. He then engaged in BSc. Applied Physics (Hons) at Universiti Tun Hussein Onn Malaysia, Johor, Malaysia, and graduated with a first-class degree in 2019. He was provided two modules, "The Questions of Mechanic Physics" and "Vibration and Waves," for the Physics students who take BWC10103 and BWC10403 courses, respectively. Also, during his bachelor's degree, he was selected among Malaysian by Akademi Sains Malaysia (ASM) and the National Centre of Particle Physics to participate in an internship bimonthly at the European Organisation of Nuclear Research (CERN), Geneva, Switzerland, in 2018. He was inculpated at Antiparticle Decelerator (AD) department in ALPHA Experiment (Antihydrogen Laser PHysics Apparatus), which scrutinises antihydrogen behaviour. He was involved in constructing, assembling, and installing numerous microchannel plate power supplies and circuit breakers for the ALPHA-g instrument, which studies the gravitational effect on antihydrogen. He returned to UTHM with the canvas of Particle Physics knowledge and encompassed in the BSc. Applied Physics as an unsanctioned tutor in Statistical Physics (BWC30103) and Quantum Physics (BWC20803 & BWC32203) courses. He lighted up the new physics and the current industrial physics to students since the wisdom of the quantum world nowadays stretches far and wide, thus, will be our future science. He then signed up MSc at the UTHM, which investigated the quantum dots applied on the solar cell to improve the light-matter interaction via numerical simulation Finite Element Method using COMSOL Multiphysics.