THEORETICAL AND EXPERIMENTAL INVESTIGATIONS OF LEAD CHALCOGENIDES QUANTUM CONFINED STRUCTURES FOR SOLAR CELL APPLICATION

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I hereby declare that the work in this thesis is based on my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at Universiti Malaysia Pahang or any other institutions.

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ABSTRAK

Sel suria mendapat perhatian yang meluas disebabkan oleh reka bentuknya yang ringkas dan mempunyai persamaan dengan sel suria terpeka pewarna (DSSC), yang mana QCS menggantikan molekul pewarna. QCS mampu menghasilkan lebih dari satu eksiton dengan penyerapan tenaga foton tunggal yang mencukupi (≥ dari jurang tenaga QCS) iaitu *multiple exciton generation* (MEG). Secara teori, mekanisma MEG ini mampu meningkatkan kecekapan penukaran fotovoltaik (PCE) bagi sesebuah QCSC ≥ 60%, namun QCSC hanya merekodkan PCE yang < ~16.6% secara praktikal. Penyelidikan kedoktoran ini bertujuan untuk, (i) mengkaji kesan penjajaran tahap tenaga antara orbital molekul tak berisi terendah fluorofor ($LUMO_{fluorofor}$) dengan jalur konduksi minimum MOS (CBM_{MOS}) terhadap kecekapan suntikan elektron dari fluorofor ke MOS, (ii) menentukan geometri QCS plumbum kalkogen (< jejari Bohr eksiton) yang mempunyai ciri MEG menggunakan *ab-initio* teori fungsian kepadatan (DFT), (iii) mengenalpasti geometri-geometri filem nipis plumbum kalkogen yang mampu disintesis menggunakan alat penyejatan haba tervakum (TE), dan (iv) mengkaji kesan penambahan karbon teraktif (AC) terhadap morfologi dan sifat optoelektronik plumbum sulfida (PbS) yang dihasilkan menggunakan alat TE serta kecekapan suntikan elektron keadaan teruja dari PbS ke MOS. Hasil dapatan kajian menunjukkan penjajaran tahap tenaga yang baik antara $LUMO_{fluorofor}$ (-4.0 eV) dengan jalur konduksi minimum MOS (CBM_{MOS} = -4.1 eV) mampu menyokong suntikan elektron keadaan teruja dari fluorofor ke MOS dengan kecekapan setinggi 97%. Geometri struktur PbS, PbSe dan PbTe yang mempamerkan ciri MEG telah dikenalpasti iaitu $(PbS)_{40}$, $(PbS)_{74}$, $(PbS)_{80}$, $(PbSe)_{16}$, $(PbSe)_{30}$, $(PbSe)_{32}$, $(PbSe)_{50}$, $(PbSe)_{74}$, $(PbTe)_{12}$, $(PbTe)_{16}$, $(PbTe)_{44}$, $(PbTe)_{50}$ dan $(PbTe)_{74}$ dengan saiz 3.49 nm, 4.86 nm, 4.58 nm, 2.63 nm, 3.20 nm, 3.29 nm, 4.03 nm, 5.02 nm, 2.52 nm, 2.69 nm, 3.90 nm, 4.16 nm dan 4.84 nm. Sifat optoelektronik QCS $(PbS)_{80}$, $(PbSe)_{30}$ dan $(PbTe)_{50}$ yang ditentukan menggunakan pengiraan *ab initio DFT* adalah menyamai sifat optoelektronik filem nipis PbS, PbSe dan PbTe; berdasarkan perbandingan antara puncak eksitonik pertama bagi filem nipis (morfologi nano-sfera) dengan model realistik PbS, PbSe dan PbTe dengan kesamaan 92.93%, 99.38% dan 95.49%. Morfologi nano-tiub PbS berjulat saiz 41-76 nm dihasilkan dengan pertambahan AC dengan luas permukaan 80 m^2/g (AC80). Nano-helaian PbS berjulat saiz 36-95 nm dihasilkan dengan pertambahan AC dengan luas permukaan 650 m^2/g (AC650). Nano-helaian PbS berjulat saiz 33-63 nm dihasilkan dengan pertambahan AC dengan luas permukaan 1560 m^2/g (AC1560). Sifat optoelektronik filem nipis PbS yang difabrikasi dengan pertambahan AC80, AC650 dan AC1560 ini menyamai sifat optoelektronik model realistik $(PbS)_{80}$ berdasarkan analisa puncak eksitonik pertama dengan kesamaan 90.1%, 96.1% dan 92.8%. Kecekapan suntikan elektron keadaan teruja dari PbS-AC80, PbS-AC650 dan PbS-AC1560 ke MOS adalah 18.48%, 62.71% dan 87.18%. Sebagai kesimpulan, filem nipis PbS yang mengandungi QCS bermorfologi nano-sfera serta mempunyai ciri MEG boleh dihasilkan menggunakan alat TE tanpa pertambahan AC.

ABSTRACT

Solar cell has gained much attention due to its simple design and similarity to dye sensitized solar cells (DSSC), in which the QCS replaces the dye molecules. The QCSs are able to yield more than one exciton upon absorption of a single photon with sufficient energy, a multiple exciton generation (MEG). Theoretically, MEG could increase the efficiency of a PV device ≥ 60%, however QCSCs could deliver an insignificant PV conversion efficiency (PCE) of only ca. 16.6%. This doctoral research therefore aims to: (i) investigate the effect of energy level alignment of the lowest unoccupied molecular orbital of the fluorophore ($LUMO_{fluorophore}$), with the conduction band minimum of MOS (CBM_{MOS}) on the electron injection efficiency from the fluorophore to the MOS, (ii) determine the geometry of lead chalcogenides QCS (< their exciton Bohr radius) that would exhibit MEG using ab-initio density functional theory (DFT) calculations, (iii) identify the simulated geometries of lead chalcogenides that could be synthesized using a vacuum thermal evaporator (TE) and (iv) investigate the effect of the addition of activated carbon (AC) on the morphology and optoelectronic properties of the lead sulphide (PbS) fabricated using a vacuum TE, and the electron injection efficiency from the fluorophore to the MOS. The results of the study show that the ideal energy level alignment between $LUMO_{fluorophore}$ (-4.0 eV) and CBM_{MOS} (-4.1 eV) supported an efficient electron injection from the fluorophore to the MOS, with an injection efficiency as high as ca. 97%. The structural geometry of PbS, PbSe and PbTe that exhibit MEG were identified viz., $(PbS)_{40}$, $(PbS)_{74}$, $(PbS)_{80}$, $(PbSe)_{16}$, $(PbSe)_{30}$, $(PbSe)_{32}$, $(PbSe)_{50}$, $(PbSe)_{74}$, $(PbTe)_{12}$, $(PbTe)_{16}$, $(PbTe)_{44}$, $(PbTe)_{50}$ and $(PbTe)_{74}$ with the size of 3.49 nm, 4.86 nm, 4.58 nm, 2.63 nm, 3.20 nm, 3.29 nm, 4.03 nm, 5.02 nm, 2.52 nm, 2.69 nm, 3.90 nm, 4.16 nm and 4.84 nm respectively. The optoelectronic properties of $(PbS)_{80}$, $(PbSe)_{30}$ and $(PbTe)_{50}$ QCS that were obtained from ab-initio DFT calculations were in good agreement the PbS, PbSe and PbTe thin films; which compared based on the first excitonic peaks of the fabricated thin films (nano-sphere morphology) to the PbS, PbSe and PbTe realistic cluster models, which resulted in similarities of 92.93%, 99.38% and 95.49% respectively. The PbS nano-tubules with a size range of 41-76 nm were yielded after the addition of AC with a specific surface area of 80 m^2/g (AC80). PbS nano-sheets with a size range of 36-95 nm were yielded after the addition of AC with a specific surface area of 650 m^2/g (AC650). PbS nano-sheets (size range: 33-63 nm) were yielded after the addition of AC with a specific surface area of 1560 m^2/g (AC1560). Optoelectronic properties of the fabricated PbS thin films with the addition of AC80, AC650 and AC1560 were similar to that of the $(PbS)_{80}$ realistic model; determined based on the positions of the first excitonic peaks, which recorded 90.1%, 96.1% and 92.8% of similarity, respectively. The electron injection efficiencies from PbS-AC80, PbS-AC650 and PbS-AC1560 conjugates to the MOS were determined to be 18.48%, 62.71% and 87.18%, respectively. In conclusion, a PbS thin film possessing a nano-sphere morphology and exhibiting MEG could be fabricated using TE without the addition of AC.

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