From Diameter Distribution to Photoluminescence: Graphene Quantum Dots(GQDs)

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Introduction

Fig 1: color emission of quantum dots and its application in television

- There is always a relation between the size of a particle and its bandgap: E(R)
- The smaller the GQDs, the larger the bandgap.

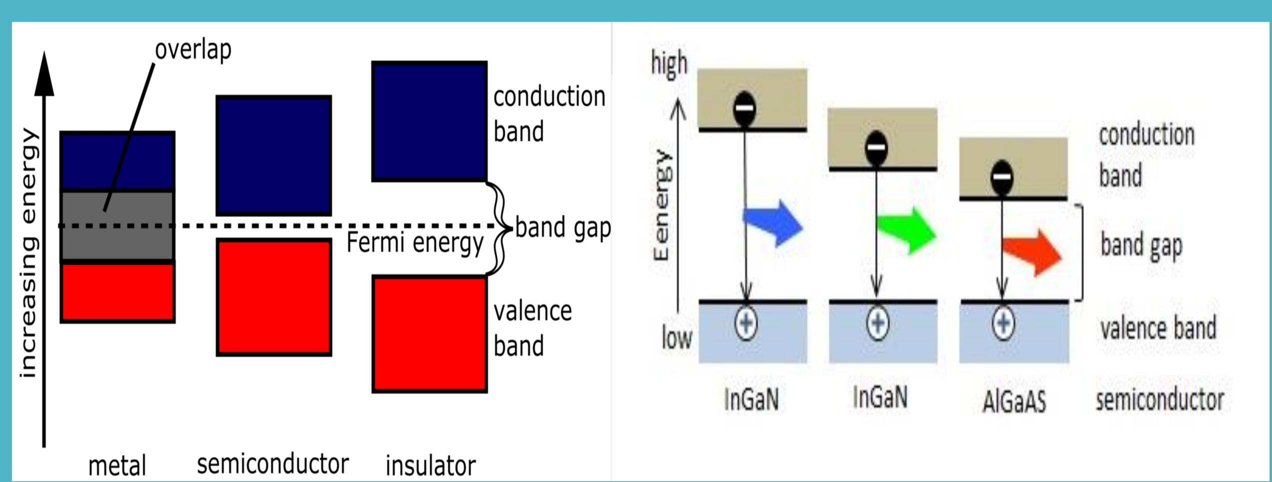

Fig 2: Mechanism of bandgap energy and photo-responses

- It is a banned gap!
- The energy of the light emitted is also equal to the energy of bandgap.

Photoluminescence (PL)

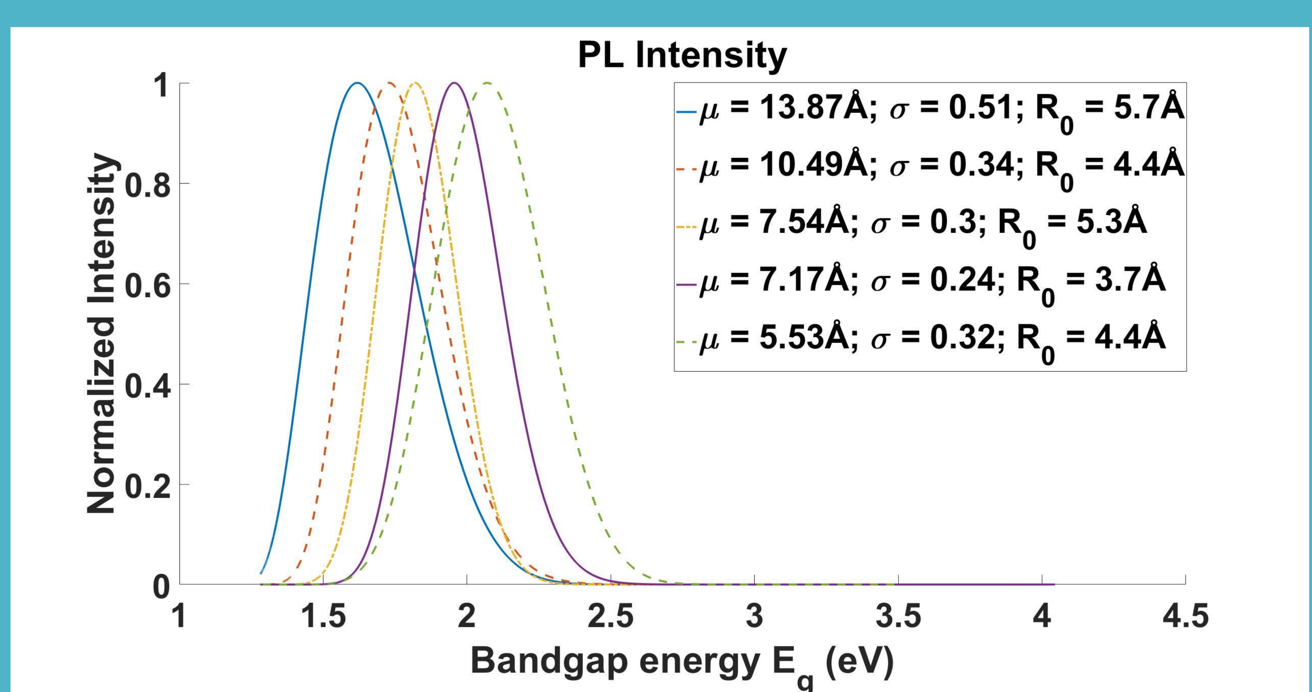

Fig 3: Simulated photoluminescence of GQDs with distinctive particle sizes distribution.

Keys to understand PL:

- Peak position: color of the emission
- Width: purity of the emission
- Shape: asymmetric shape due to log-normal particle-size distribution

Model

$$S(E) = c(E_{exc})\ \alpha(E - E_{exc})\ P(E)$$

c : A constant determined by excitation energy.

$\alpha(E - E_{exc})$**:** Absorption coefficient of a particle with bandgap E.

$P(E)$**:** Distribution of bandgap derived from distribution of radius.

$$P(E) = D(R_{(E)})\frac{1}{n}\left|\frac{R_{(E)}}{E - E_g^0}\right|, \qquad E_{(R)} = \frac{\gamma}{R^n}$$

R(E): the radius of a particle that has bandgap E : inverse of E (R)

$$\begin{cases} E^z_{(R)} = \dfrac{\gamma_z}{R^{n_z}} \\ E^a_{(R)} = \dfrac{\gamma_a}{R^{n_a}} \end{cases}$$

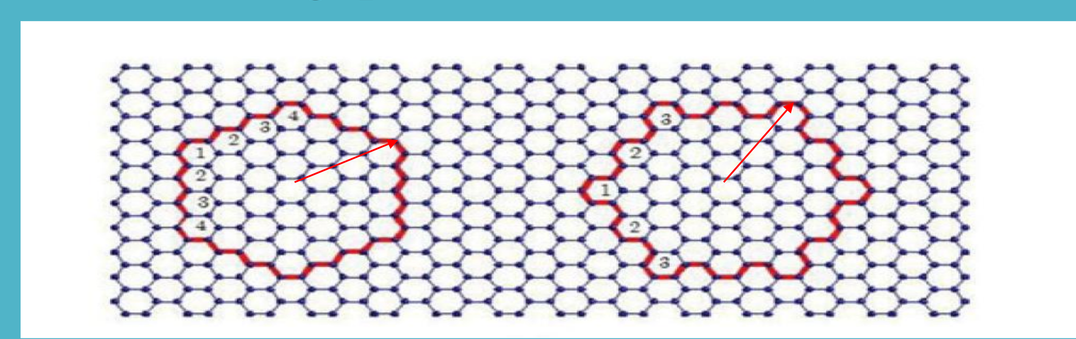

Fig.4: Schematic diagram of Zigzag GQDs (left) and Armchair GQDs (right). The arrow denotes the definition of radius in each case[1].

Benchmarking

Known: Experimental data of S(E); Theoretical prediction of E(R).
Assumptions: Absorption coefficient is constant; $E_g^0 = 0$ for GQDs .
Goal: Fit S(E) to data; look for best-fit γ and n.
Expectation: A mixture of Zigzag and Armchair GQDs: $E^z_{(R)} < E_{(R)} < E^z_{(R)}$.

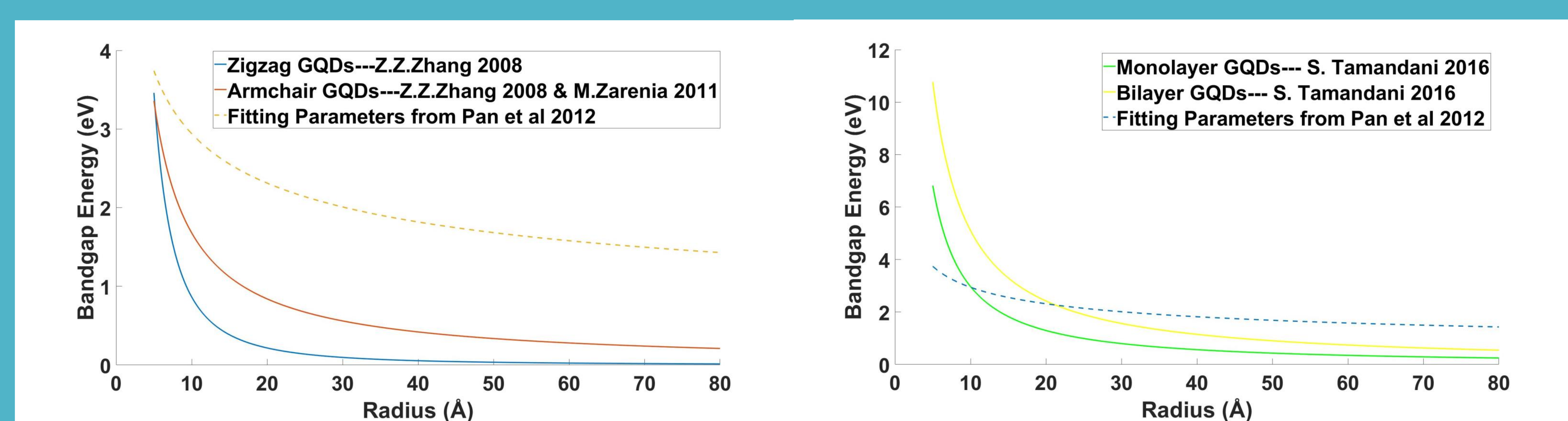

Fig 5: Comparison between our prediction and theoretical calculations for Left: single layer GQDs; Right: single/ bilayer GQDs

Limitations

- Functional groups terminating the carbon bond at the edge of GQDs[2,3]
- Inhomogeneous layer number[3]
- Absorption effect

References

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Acknowledgements

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