Quantum Confinement of Electron−Phonon Coupling in Graphene Quantum Dots

Marios Zacharias[a,*] and Pantelis Kelires[a]

[a] *Department of Mechanical and Materials Science Engineering, Cyprus University of Technology, P.O. Box 50329, 3603 Limassol, Cyprus*

**Now at FOTON Institute, INSA Rennes, France*

Corresponding author email: pantelis.kelires@cut.ac.cy

On the basis of first-principles calculations and the special displacement method, we demonstrate the quantum confinement scaling law of the phonon-induced gap renormalization of graphene quantum dots (GQDs) [1]. We employ zigzag-edged GQDs with hydrogen passivation and embedded in hexagonal boron nitride. Our calculations for GQDs in the sub-10 nm region reveal strong quantum confinement of the zero-point renormalization ranging from 20 to 250 meV. To obtain these values we introduce a correction to the Allen−Heine theory of temperature-dependent energy levels that arises from the phonon-induced splitting of 2-fold degenerate edge states. This correction amounts to more than 50% of the gap renormalization. We also present momentum resolved spectral functions of GQDs, which are not reported in previous contributions. Our results lay the foundation to systematically engineer temperature-dependent electronic structures of GQDs for applications in solar cells, electronic transport, and quantum computing devices.

[1] M. Zacharias and P. C. Kelires, *J. Phys. Chem. Lett.* 2021, 12, 9940-9946.