

## Tuning the Kataura Plot (II)

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Energy separations of van Hove singularity peaks of single-walled carbon nanotubes (SWNTs) plotted against diameter is called Kataura plot [1] and conveniently used for interpretation of resonant Raman scatterings, optical absorption and fluorescence spectroscopy. However, the original Kataura plot calculated by a simple tight-binding (TB) method only qualitatively agrees with experimental results. Recently, Weisman and Bachilo [2] suggested so-called an “empirical Kataura plot” based on fluorescence and resonance Raman measurements. Even though the apparent agreement to observed spectroscopic results seems satisfactory with this plot, an improvement and modified assignment may be possible with better theoretical background. Here, we suggest a Kataura plot based on higher level theoretical calculation and try to tune it for better experimental fit. The energy dispersion of graphene was calculated with local density approximation (LDA) level and with GW approximation. The joint density of states (JDOS) and Kataura plots were generated as in Fig. 1. The Kataura plot based on graphene with GW approximation is very much similar for  $E_{22}^s$ .

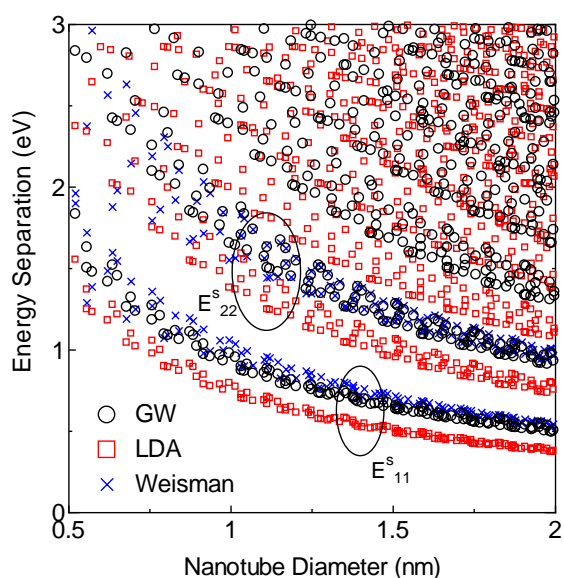


Fig. 1 Comparison of Kataura Plots

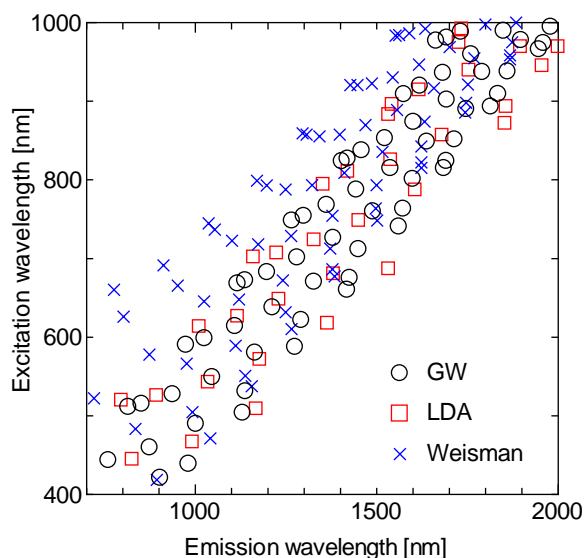


Fig. 2 Plot of first band-gap vs. second band-gap in comparison with fluorescence measurements.

[1] H.Kataura et al., Synth. Met. 103 (1999) 2555.

[2] R.B. Weisman, S.M. Bachilo, Nano Letters, 3 (2003) 1235.

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