

Kataura plot based on GWA graphene dispersion

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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.

In the last symposium, we have compared Kataura plots based on higher level theoretical dispersion relations. The energy dispersion of graphene was calculated with π - σ tight-binding model, with local density approximation (LDA) level and with GW approximation. Among them, the Kataura plot based on a graphene dispersion with GW approximation was very much similar to the Weisman's "empirical Kataura plot" [2] as shown in Fig. 1 and Fig. 2.

The Kataura plot based on GWA dispersion will be compared with fluorescence measurements in various environments, and recent Raman measurements from tuned excitation energy.

[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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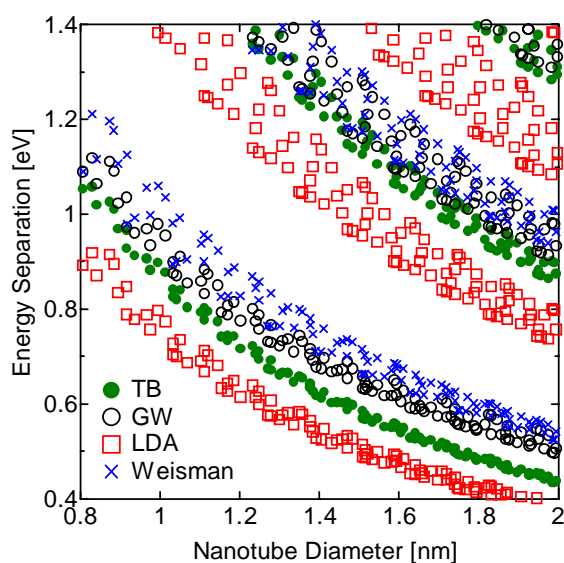


Fig. 1 Comparison of Kataura Plots

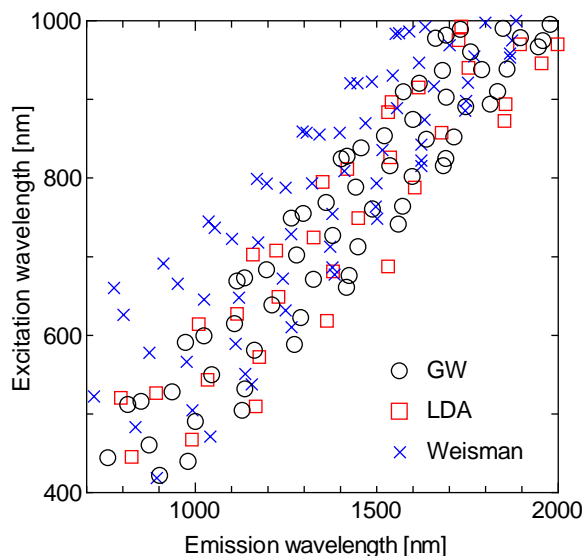


Fig. 2 Plot of first band-gap vs. second band-gap in comparison with fluorescence measurements.