# Tuning the Kataura Plot

○Satoshi Ogawa[1], Susumu Okada[2] and Shigeo Maruyama[1]

*1) Department of Mechanical Engineering, The University of Tokyo*
*7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*
*2) Institute of physics and center for computational physics, University of Tsukuba*
*Tennodai, Tsukuba 305-8751, Japan*

The Kataura plot [1] is very useful for analyzing optical spectroscopic results of SWNTs (resonance Raman spectroscopy and fluorescence spectroscopy); however, the 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 agreement to observed spectroscopic results is much better with this plot, an improvement 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 electric density of states and a Kataura plot were generated as in Fig. 1. Compared to TB based one, enhanced scatterings due to the trigonal warping effect was observed. The scattering width approximately agrees with the spectrofluorimetric results as in Fig. 2. The higher level calculation of energy dispersion and direct TB calculation of small diameter nanotube geometries are also in progress.

[1] H.Kataura et al., Synth. Met. 103 (1999) 2555.
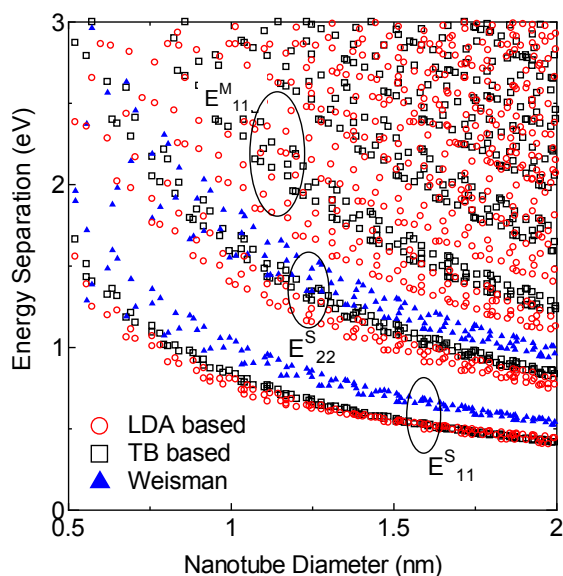[2] R.B. Weisman, S.M. Bachilo, Nano Letters, 3 (2003) 1235.
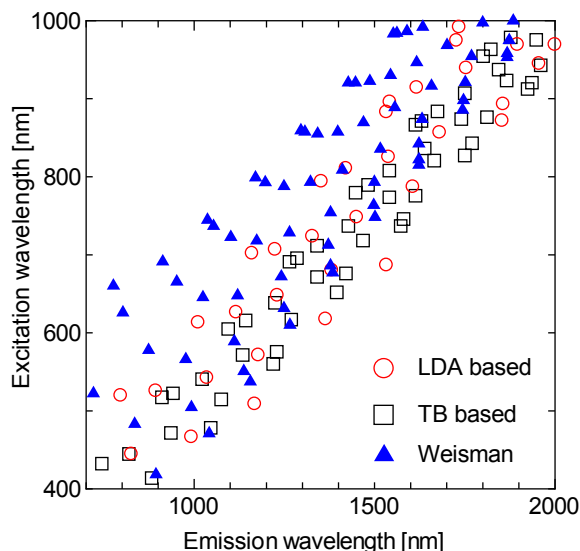
Fig. 1 Comparison of Kataura Plots



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

Corresponding Author: Shigeo Maruyama
E-mail: maruyama@photon.t.u-tokyo.ac.jp
Tel/Fax:+81-3-5800-6983