

Kataura plot based on GWA graphene dispersion

○Mototeru Oba¹⁾, Susumu Okada²⁾, Takashi Miyake³⁾, and Shigeo Maruyama¹⁾

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 Sciences, University of Tsukuba
1-1-1 Tennodai, Tsukuba 305-8751, Japan

3) Department of Physics, Tokyo Institute of Technology
2-12-1 Oh-okayama, Meguro-ku, Tokyo 152-8551, Japan

Peaks of joint density of states (JDOS) 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.

There are two ways to calculate the plot: one is to calculate SWNT energy band directly; another is to use zone-folding approximation to the calculated energy band of a graphene sheet. Since the former is too heavy to calculate with *ab-initio* calculation such as local density approximation (LDA) and GW approximation (GWA), a comprehensive technique to compensate the curvature effect on zone-folding method (Fig. 1) is desired.

Here, Kataura plot calculated from geometry optimized nanotube structure was compared with the simple zone-folding approximation within Hamada-TB [2] level as in Fig. 2. After the full understanding of geometry effect and deviation of compensation function, this compensation function was applied to the dispersion relation of graphene calculated with GWA.

- [1] H.Kataura et al., Synth. Met. 103 (1999) 2555.
[2] N.Hamada et al., Phys. Rev. Lett. 68 (1992) 1579.

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

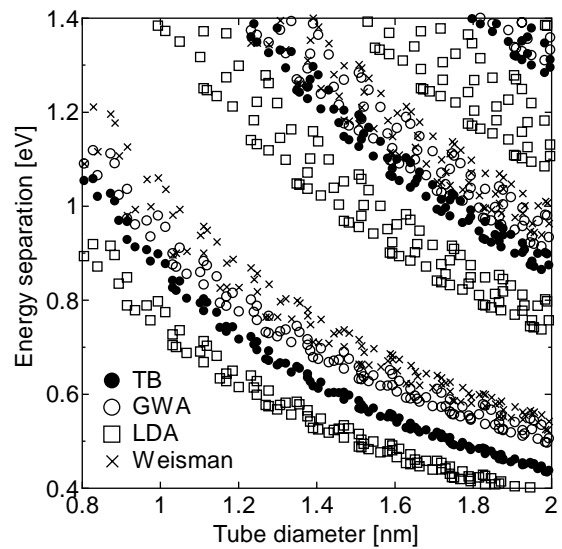


Fig. 1 Kataura plot from zone-folding of graphene with GWA, LDA, TB models.

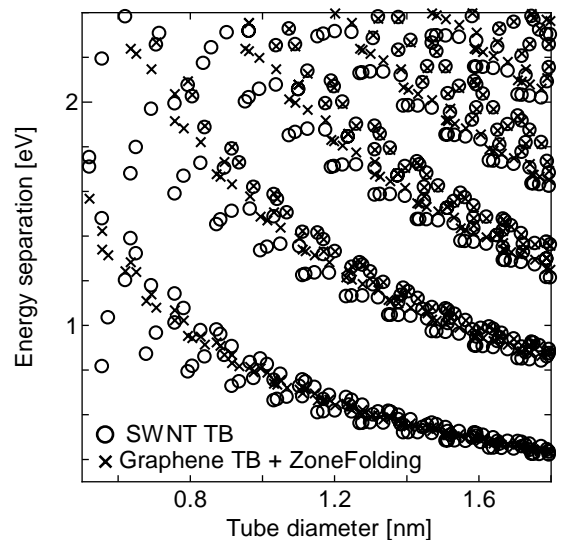


Fig. 2 Curvature effect in Kataura plot examined by Hamada-TB level.