

Abstract Submitted
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WKB modeling of single molecular transport and Molecular Nanometrology¹ VLADIMIR BURTMAN, Physics and Geophysics Department, University of Utah, SLC, ANDREI V. PAKOULEV, Department of Chemistry, University of Wisconsin, Madison — Wentzel–Kramers–Brillouin (WKB) approach to model transport mechanism in molecular nanostructures is discussed in content of molecular nanometrology. Two WKB models, direct tunneling (Simmons model) and field emission tunneling (Fowler–Nordheim tunneling), could be used to model conductivity in single molecular structure at low and elevated biased. Potentially, Simmons model could extract two molecular barriers, one for electrons and one for holes from conductivity spectra. Following this assumption electrical and optical gap-probed molecular nanometrology (GMN) could be developed. The main GMN principle is the small difference between the values of the HOMO-LUMO energy gap detected by electrical and optical measurements. We will compare experimentally derived electrical and optical probed gap and energy offsets between E_F and nearest molecular orbital to discuss applicability and feasibility of this approach.

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