

Abstract Submitted
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The zero-voltage conductance of nano-graphenes: Simple rules and quantitative estimates¹ MATTHIAS ERNZERHOF, YONGXI ZHOU, University of Montreal, DIDIER MAYOU, Institut Néel, Grenoble — Zero-dimensional graphenes, also called nano-graphenes (*NGs*), consist of fragments of graphene with a finite number of hexagons. *NGs* can be viewed as a subset of the polycyclic aromatic hydrocarbons (PAHs) that continue to attract chemists attention. We develop a simple theory for the ballistic electron transport through *NGs* which combines elements of the electronic structure theory of graphene, intuitive methods for the calculation of the molecular conductance, and chemical concepts such as Kekulé structures. This theory enables one to analyze the relation between the structure of *NGs* and their conductance. General formulas and rules for the zero-voltage conductance as a function of the contact positions are derived. These formulas and rules require at most simple paper and pencil calculations in applications to systems containing several tens of carbon atoms.

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Matthias Ernzerhof
University of Montreal

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