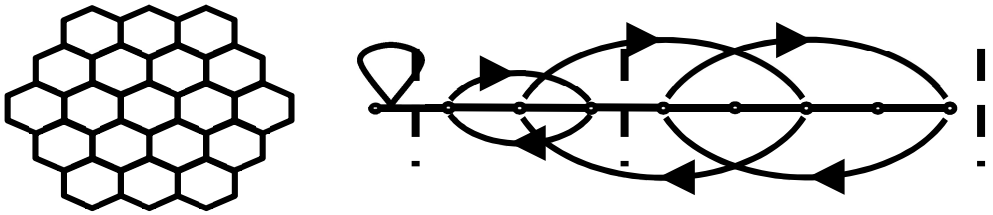
Approach to zero band gap graphene sheets: A graph theoretical analysis

Bankim Chandra Ghosh
Department of Chemistry, Durgapur Government College, J. N. Avenue, Durgapur-713214



Abstract

A method of construction of graphs for extended graphene sheets of the formula , maintaining six-fold symmetry has been developed. It has been shown that their adjacency matrices, which are of size , can be reduced to matrices by exploring rotational symmetry and the reduced matrix can be easily written down as the adjacency matrix of a directed graph with vertices (called 'reduced graph' in this article). A scheme for drawing the reduced graph is devised and from this the graph eigenvalues can be easily determined. It has been shown that the HOMO-LUMO energy gap of the π-MOs decreases as *n* increases, and an almost gapless graphene sheet , where resonance integral between two adjacent –C atoms) begins to form at carbon atoms arranged in a 2-dimensional hexagonal lattice.

Key words: Graph theory, graphene, reduced graph, zero band gap