Construction of upper bounds of the HOMO-LUMO spectral gaps by semidefinite relaxation techniques

Soňa Pavlíková

Slovak University of Technology

`sona.pavlikova@stuba.sk`

An important application of graph theory in quantum chemistry is based on the fact that the energy of the highest occupied molecular orbital (HOMO) and of the lowest unoccupied molecular orbital (LUMO) of a molecule correspond, respectively, to the smallest positive and the largest negative eigenvalue of a graph representing the molecule; the difference of these eigenvalues is known as the HOMO-LUMO spectral gap.

In our contribution we study the HOMO - LUMO spectral gap of weighted graphs. In particular, we focus constructions of new graphs from old by 'bridging' two input graphs over a common bipartite subgraph, with the aim to maximize the spectral gap with respect to the structure of the ingredients. Among the tools we use estimates of the spectrum of the inverse of a block matrix consisting of adjacency matrices of input graphs on its block diagonal and the adjacency matrix of the bridging graph as off-diagonal blocks; maximization of the HOMO-LUMO gap turns out to be equivalent to minimization of the sum of largest and smallest eigenvalues of the inverse of the block matrix. An upper bound on the gap is then be obtained by semidefinite programming.

This a joint work with Daniel Sevcovic.