

Seminar za kombinatornu i diskretnu matematiku

7.6.2018. Ivana Zubac (Sveučilište u Mostaru): **Partition of π -electrons among the faces of polyhedral carbon clusters**

Abstract

We apply the concepts of importance and redundancy to compute and analyze the partition of π -electrons among faces of actual and potential polyhedral carbon clusters. In particular, we present explicit formulas and investigate asymptotic behavior of total and average π -electron content of all faces of prisms and n -barrels. We also discuss the observed deviations from the uniform distribution and show that the patterns of net migration of π -electrons differ from those computed for narrow nanotubical fullerenes. Some possible directions of future work are also indicated.