United Nations
Educational, Scientific and
Cultural Organization

II WORKSHOP ON UNESCO-HP
"BRAIN GAIN INITIATIVE"
In Conjunction with:
GraphMasters
http://www.graphtheorygroup.com/graphmasters/

Wiener index and Nanotechnology

The UNESCO-HP "Brain Gain Initiative" project establishes e-infrastructure Grid Network that will facilitate links with the Diaspora, enhance brain gain and strengthen university teaching and research capabilities in Africa and the Arab region. One of the objectives of the UNESCO-HP project is to bring together different researchers who will be willing to run research projects in close collaboration with experts in the Diaspora of African region. The Second workshop on UNESCO-HP "Brain Gain Initiative" will describe the features of this network that will enable researchers to carry out collaborative research with experts in the Diaspora. In addition, a few research problems on nanotechnology will be discussed and these problems will be potential research topics for research collaboration with Diaspora.

Nanotechnology is the next industrial revolution that is expected to radically transform the computer industry. Nano-computing which is the computational aspects of nano architectures is an emerging technology and is at the early stage of its development. One of the most widely known topological descriptor is the Wiener index named after chemist Harold Wiener. The *Wiener index* is used to study the relation between molecular structure and physical and chemical properties of certain hydrocarbon compounds. It is defined as the sum of the distances between every pair of vertices of G. It is employed to predict boiling point, molar volumes and large number of physico-chemical properties of alkanes. Wiener index correlates well with many physico chemical properties of organic compounds and as such has been well studied over the last quarter of a century.

Wiener index of chemical compounds had been computed using brute force method based on distance matrix. Researchers made some attempts to device efficient technique to find Wiener index of chemical compounds. There was no efficient unified technique discovered to compute Wiener index. This motivated Bojan Mohar and Tomaž Pisanski to pose an open problem "is there an algorithm for general graphs that would calculate the Wiener index without calculating the distance matrix?" This open problem was posed in 1988 in Journal of Mathematical Chemistry. It remains unsolved until now. In this workshop we discuss possible strategies to solve this two-decade open problem.