



KEMIJSKI INŠTITUT

Vabilo na Preglov kolokvij / Invitation to the Pregl colloquium

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Velika predavalnica Kemijskega inštituta /  
Great Lecture Hall, National Institute of Chemistry;  
Hajdrihova 19, Ljubljana, Slovenia

**Modern Approaches to  
Hückel Molecular Orbital Approach in Chemistry**

The Hückel Molecular Orbital (HMO) Approach is 85 years old. The discovery of graphene and quantum dots derived from it has increased the interest in the use of HMO. In this colloquium I will start by a historical introduction of the developments of the HMO method, its uses in chemistry and in physics and the seminal contributions to its development by many bright scientists. Then, I will focus of recent developments on HMO to problems of great theoretical and practical relevance in chemistry and material sciences. First, I will develop a mathematical approach to illustrate the meaning of the HMO total energy of a molecule. In a similar way I will give a structural interpretation of the electron-density matrix of the HMO method and produce new geometric parameters that explain the known relation between bond orders and bond lengths in conjugated molecules. Finally, I will concentrate on the explanation of the phenomenon of destructive quantum interference (QI). In this case I will give a mathematical approach to the study of the Green's function of HMO and will show its connection to QI and several existing physical approaches. I will illustrate all the subjects with a large variety of examples to make easy the understanding of the concepts involved.

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Vljudno vabljeni / Kindly invited