Dear Colleagues,

This is for your kind information that Prof. M. Springborg, Head of the Physical and Theoretical Chemistry Division, University of Saarland, Saarbrücken (Germany) will be delivering 3rd Pran Nath Vohra Lecture under the aegis of Pran Nath Vohra Lectures in thrust areas in Chemistry as per following schedule:

Date: **November 21, 2017**

Time: **11.30 A.M.**

Venue: **Seminar Hall, Department of Chemistry, P.U. Chandigarh**

Topic: **On the Theoretical Optimization of Properties**

Kindly make it convenient to attend.

The abstract of the talk is enclosed herewith for your kind reference.

Chairman

On the Theoretical Optimization of Properties

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During the last few decades, theoretical calculations have become of increasing importance in providing supporting and complementary information to what is provided by experiment. On the one side, such studies can help in the interpretation of experimental results and, on the other side, through such calculations a first screening of systems can be carried through, ultimately allowing for reducing the synthetic work in the lab. In all those cases, the conventional approach is to start with a realistic structure for the system of interest whose stoichiometry is known, subsequently let the system relax to a close structure of a local totalenergy minimum, and finally for this calculate the properties of interest. The situation is different when essentially nothing is known about the structure of the system of interest. This is, e.g., the case for clusters and nanoparticles. For such systems, specialized theoretical methods that aim at identifying the global total-energy minima have to be applied. Another challenge is to identify molecular systems with optimal properties without specifying the stoichiometry.

In the present contribution we shall at first demonstrate how methods based on genetic algorithms can be used in optimizing the structure of nanoparticles. Subsequently, related methods will be used in identifying molecular systems with optimal properties, whereby, as a playground system, mixed Ge-Si clusters with optimal properties in solar-energy harvesting shall be identified. The purpose of this method, PooMa, is to provide useful information for experiments about interesting systems with predefined properties. It is based on many approximations and is not aimed at providing exact information on any detail. PooMa is developed as a simple, efficient method that does not rely on heavy computations or results from, e.g., high-throughput studies.

PooMa: M. Springborg, S. Kohaut, Y. Dong, and K. Huwig: *Mixed Si-Ge clusters, solar-energy harvesting, and inverse-design methods,* Comp. Theo. Chem. **1107** (2017) 14-22.