Structural and electronic properties of nanostructures – cluster model

Materials in the nanoscale are still increasingly used in many applications. It is due to their unique properties, completely different from the native materials, arising from their size limitation. Moreover, doping, surface modification, and shape tailoring may change the physical properties of nanocrystals. Semiconducting nanoparticles are popularly used in photovoltaic and photocatalytic applications, where the most known are titanium oxide, zinc oxide, and bismuth vanadate based materials. Computer simulations and quantum chemical calculations can explain the nature of photoinduced phenomana occurring in the mentioned materials, but the methodology of the computer approach to this problem should be implemented.

The lecture will present a comprehensive overview of structural and electronic properties of nanostructures investigated using the cluster model approach within quantum-chemical calculations. Particular attention will be paid to the applicability of finite-size models in describing systems that inherently exhibit extended or periodic character, such as semiconductor nanostructures and hybrid materials. The cluster model enables the analysis of local structural features, electronic density distribution, and energy states with high accuracy while maintaining computational efficiency. The methodology based on quantum chemistry tools, including density functional theory (DFT) and post-Hartree–Fock methods, will be discussed in the context of predicting key properties such as band gap, charge distribution, and opical property. The lecture will also address the influence of cluster size, boundary conditions, and surface effects on the reliability of the obtained results. Examples of nanostructured and hybrid systems will be presented to illustrate how the cluster approach can be effectively applied to model charge transfer mechanisms and photoinduced processes.

The presented studies demonstrate that the cluster model constitutes a powerful and versatile tool for understanding and predicting the structural and electronic behavior of nanoscale materials, providing valuable insights for the design of advanced functional systems.