

Joint Event

^{2nd} International Conference on Nanomaterials and Nanotechnoloav

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22nd International Conference on

Advanced Nanoscience and Nanotechnology

May 16-17, 2019 | Prague, Czech Republic

Bandgap tunability in one dimensional system

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For optoelectronic applications of low dimensional materials, a direct bandgap is required; but for optoelectronic applications of the same material in different wavelength range, bandgap tunability is required. Even though tunability of bandgap in direct bandgap materials carries huge potential for optoelectronic applications like LEDs and solar cells, an exhaustive formulation for bandgap tuning is unavailable. In this article, we report broad theoretical investigations using periodic potential profiles for direct bandgap one-dimensional isomeric systems having the same functional groups. We derived all possible correlations between bandgaps of one-dimensional isomeric systems using two parameters, width and depth of the deepest potential well at global minimum. The derived correlations are verified for known synthetic as well as natural polymers (biological and organic) and also for other one-dimensional direct bandgap systems. We have demonstrated bandgap tuning simply by modifying the potential profile on changing the position of the functional group in a periodic supercell.

This insight would greatly help experimentalists in designing new isomeric systems of different bandgap values from a direct bandgap polymer or a one-dimensional inorganic system for its optoelectronic applications.

Speaker Biography

Rakesh Kumar is an assistant professor in the department of Physics at IIT Ropar, India. In 2006, he received his PhD degree from Indian Institute of Technology Bombay, where he worked on superconductivity and magnetism. Thereafter, he joined Tata Institute of Fundamental Research, Mumbai as a visiting fellow, where he continued his research work on magnetic materials. In 2007, he moved to University of Peirre and Marie Curie, Paris, France to work on graphene and other twodimensional layered materials like InSe, NbSe₂, BSCCO superconductors and Bismuth. He worked on fabrication as well as electrical characterization of Field Effect Transistors (FETs). His current research interests focused on theoretical and experimental investigations of low dimensional materials and the involved Physics towards its electronic applications.

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