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A Theoretical Study of Copper Sulfide Nanoalloy Clusters: Density Functional Approach

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Importance of Nano clusters of Copper sulfides (CuS) is well known due to its interesting properties. Our group have studied nanoalloy clusters of (CuS)n; (n = 1–8) in terms of Conceptual Density Functional Theory (CDFT) based descriptors, aiming to explore its electronic and other properties. Global DFT based descriptors have been computed for ground state configurations and low-lying isomers of (CuS)n clusters. Our computed HOMO-LUMO energy difference, lying in the range of 1.25–3.53 eV, indicate possibility of utilization of (CuS) n clusters as renewable energy sources specially in photocatalysis and solar cell applications. A statistical regression analysis has been made between electronic and photo-catalytic properties of copper-sulfide clusters with their computational counterparts. The close agreement between experimental and computed data strengthens our analytical approach.

Speaker Biography

Tanmoy Chakraborty, PhD, is associate professor in the Department of Chemistry at Manipal University Jaipur, India. He has been working in the challenging field of computational and theoretical chemistry for last nine years. He has completed his PhD from the University of Kalyani, West-Bengal, India, in the field of application of QSAR/QSPR methodology in the bioactive molecules. He has published a large number of international research papers in peer-reviewed international journals with high impact factors. In addition, he has edited a number of research books. He served as an international Editorial board member of the International Journal of Chemoinformatics and Chemical Engineering. He is the recipient of prestigious Parameswar Mallik Smawarak Padak, from Hooghly Mohsin College, Chinsurah (University of Burdwan), in 2002.

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