Electronic Structure and the Origin of Metal-Insulator Transition in Bi-Based Charge Ordered Systems

Indra Dasgupta

School of Physical Sciences
Indian Association for the Cultivation of Science
Jadavpur, Kolkata-700032, India

Metal-insulator transition driven by charge ordering or charge disproportionation have attracted considerable attention both in experimental and theoretical research in condensed matter physics. We shall present our results based on first principles calculations to understand the electronic structure of Bi and Ni based charge ordered systems [1] [2]. Bi and Ni have both intermetallic charge transfer degree of freedom and charge disproportionation instability along with negative charge transfer gap. Our systems show charge ordering at the Bi site and metal-insulator transition. We shall show the importance of Bi-O and Ni-O covalency in these type of systems and discuss the actual charge state of the constituent ions. Finally we shall explain the origin of the charge ordered driven metal-insulator phase transition in such systems.

[1] A. Paul, S. Bandopadhyay and I. Dasgupta *(Submitted for Publication)*

[2] Atanu Paul, Anamitra Mukherjee, Indra Dasgupta, Arun Paremkanti and Tanusri Saha-Dasgupta (*arXiv:1801.08152)*