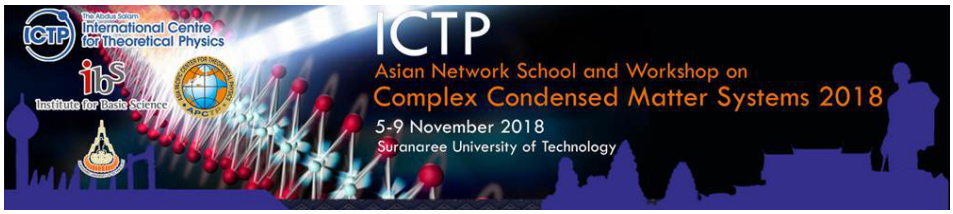

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First-Principles Electronic Structure Calculations of MgZn-based Ternaries

The present talk will discuss the computed results of electronic energy band structure, partial density states, total density of states and electronic charge density for nine MgZn-based metallic complexes: MgZnCo2, MgZnRh2, MgZnIr2, MgZnNi2, MgZnPd2, MgZnPt2, MgZnCu2, MgZnAg2, and MgZnAu2. The first principles electronic structure calculations is made by employing density functional theory as implemented in Quantum Espresso. All the nine materials belong to the cubic class of Bravais Lattice with space group Fm m (in full detail it is F 4/m 2/m) and space group number 225. The Pearson symbol for them is cF16, i.e. it is a face centred cubic system consisting of 16 atoms for complete representation of conventional unit cell. All the ternaries are found metallic by nature. The band structure is found more dispersive along the path K-Γ-L. An indirect band separation below the Fermi level is seen at around 6.23, 6.08, 6.21, 5.37, 6.27, and 6.48 eV for MgZnNi2, MgZnPd2, MgZnPt2, MgZnCu2, MgZnAg2, and MgZnAu2. The highest peak in DOS is due to d-orbitals of Zn and it is located around 7 eV below the Fermi level. The Charge density plots show that highest electron density is around Zn and lowest around Mg. The charge density between Zn and the substituted atom (Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag, and Au) is more compared to other interactions. It is also found that MgZnCu2 has 100 times more charge density at the minimum scale compared to the other eight ternaries.

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