Abstract

Cathodes are critical components of rechargeable batteries. Conventionally, the search for cathode materials relies on experimental trial-and-error and a traversing of existing computational/experimental databases. This study reports the structural, electronic, thermoelectric, thermodynamic, charge density, and orbital hybridization effects for new cathode compounds $LiXSbO_3$ (X= Ti, Ni, Mo) using Density Functional Theory (DFT). The Full Potential Linearized Augmented Plane Wave method is used to investigate these properties. The structural optimization reveals that these compounds are stable in the Orthorhombic phase with space group 47Pmmm. The electronic properties are studied to check the nature of materials. From the band gap and density of states, it reveals that these compounds have metallic nature. To study the response of the materials to temperature their thermoelectric properties like carrier concentration, electrical conductivity, See back coefficient, and thermal conductivity are studied. Results exhibit that the electrical conductivity and thermal conductivity of Ni are high as compared to other cathodes as they have more valence electrons as compared to Ti and Mo. Similarly, thermodynamics properties are used to understand, how energy flows in certain directions by understanding entropy, specific heat capacity, and Gibbs energy. As the Gibbs energy is a measure of potential, the Mo-based cathode has more negative Gibbs energy, which means it can provide high potential when used as cathode material, as compared to Ti and Ni. The magnetic moment, charge density, and Hybridization state are also used to understand the oxidation state of the transition metals. The calculated values predict that the Mo-based compounds can provide better redox reactions and can be used as better cathode material in the future.