Honeycomb Structures of Transition Metal-Group 6A Elements
CAN ATACA, HASAN SAHIN, ETHEM AKTURK, SALIM CIRACI — In this study, we investigated the structural, electronic, magnetic properties and stability of MoS$_2$ like honeycomb structures, namely MX$_2$ where M is a transition metal atom (Ti, V, Cr, Mn, Fe, Co, Ni, Nb, Mo, W) and two group (X) 6A elements (O, S, Se, Te) in a unit cell, using first-principles density functional theory. The structure consists of three layers, two for group 6A elements and one for the transition metal atom. The stabilities of various new structures are further testified by phonon dispersion analysis. Unlike graphene, some of the new honeycomb structures resulted in magnetic ground states. It is also noted that metallic honeycomb structures also exist.