Abstract
We present a theoretical model to compute the localized electronic states at the surface of an hexagonal compact packing (hcp) structures. The system under study is assimilated to a surface layer that ends a 3D semi-infinite hcp system, in [100] direction. To compute the model, we have used the phase field matching method (PFMM) along with the linear combination of atomic orbitals (LCAO) in the tight-binding approach. The PFMM helps to solve the rectangular secular equations generated by the lack of symmetry on the surface. Moreover, the localized surface states of the electrons on the surface were found by making use of the scattering reflection probabilities, as given in the Landauer and Büttiker formalism. In this work, we have studied three cases: each atom, in the surface, is described by the interaction energies of type f-, p-f- and s-p-f- coupling orbitals. Practically, our model calculations were applied to compute the localized electronic states of the following elements: (i) Gadolinium (Gd) described as f-like orbital. (ii) Lutetium (Lu) given as p-f- type orbitals. (iii) Thallium (Tl) described by s-p-f- type orbitals. The results show many localized surface branches above and down the bulk bands. Some of these states are resonant since they are located in the bulk range, and others are proper surface states since they are observed outside the bulk band range. In addition, we have investigated the relaxation effect on the surface by calculating the localized electronic surface states in the case of f-coupling orbitals. The spacing geometry caused by the relaxation on the surface has been determined by using the Molecular Dynamic algorithm. In this case, the results detail the apparition of more localized electronic states inside and outside the bulk range while integrating the relaxation effects.