DFT study of electronic, magnetic and optical properties of P_{n+1} and AlP_n (1≤ n ≤14) clusters

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In this work we have investigated the properties of pure phosphorus and aluminum doped phosphorus clusters in the range size of 2 to 15 atoms by using the first principles Density Functional Theory (DFT) within the generalized density functional approximation (GGA) implemented in SIESTA simulation package. The calculated binding energy per atom as a function of size increases as the cluster size increase which indicating that the clusters continue to gain energy during the growth process. In general the binding energies increase as the cluster size increases because the overall stability is expected to increase as the cluster grows larger and eventually reach the bulk value of binding energy in bulk crystal. The stabilities of different AlP_n clusters have been discussed in terms of their structures bond distances and the effect of the position of doping atom. The evolution of the electronic structure can be probed by calculating the characteristics of the energy gap between high occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). The theoretical HOMO–LUMO gaps are generally decreases as the cluster size increases. This indicates that the AlP_n clusters with large size seem to be approaching the gap closure characteristic of a metallic state which is enhanced by the doping Al atom. The vertical ionization potential (VIP), vertical electron affinity (VEA) and chemical hardness (η) of P_{n+1} and AlP_n are simulated theoretically, analyzed discussed for all the ground-state clusters. We obtained that the VIP values decreases as the cluster size increases indicating the high metallic character of the large size clusters. The VEA values are increased tendency with clusters sizes. This indicates that the P_{n+1} and AlP_n clusters with large sizes will liberate more energy when they capture one electron. The magnetic properties of P_{n+1} and AlP_n clusters are discussed according to the value of the total magnetic moment calculated for the lowest energies structure. The optical response of these two systems are also calculated and analysed.