On the Interaction of Beryllium atoms with Graphene Nanostructures

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Linear chains of Beryllium atoms have been shown to be local minima on the Potential Energy Surface of the isolated systems. These structures present, close to their equilibrium geometry, two edge orbitals. These orbitals are located at the two chain extremities, and give rise to two quasi-degenerated electronic states, a Singlet and a Triplet. Although these linear structures are locally stable as isolated chains, they could easily collapse into more compact, and more stable, clusters. One possibility to stabilize such structures could be via the interaction with a surface. In this context, Carbon surfaces (in particular, Graphene or Graphene fragments and Carbon Nanotubes) would be particularly appealing. As a preliminary step toward the study of Beryllium chains placed into Carbon Nanotubes, we performed a theoretical investigation of the interaction of Beryllium atoms with graphene nanostructures. In particular, rings composed of a small number of hexagonal cells (cyclic oligoacenes) have been considered in the present work.

References

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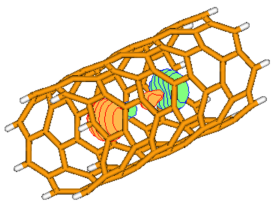

Figure 1: The Linear Be_3 inside the nanotube (8,0)