Carbon Nanotubes (CNTs) have attracted much interest because of their various properties and future applications. Although the growth mechanism of CNTs is still controversial, it is well known that using metal catalysts is one of efficient ways to grow CNTs.

In this study, we verify that Ruthenium is not an appropriate catalyst for CNT growth due to a strong interaction between carbon and ruthenium atoms based on SeqQuest quantum calculations. For this calculation a three-layered ruthenium slab (Fig 1) was used.

Fig 1. 3-layered Ru slab
(Length units are in Å)