Summary

This thesis sums up the results of our calculations on the physical properties of various single walled carbon nanotubes in a wide diameter range, focusing on small diameter tubes. Our investigations summarized here were the first systematic analysis of 40 different nanotubes, including 14 chiral tubes, on the first principles level of theory. The optimized geometry, the totally symmetric vibrational modes, and the electronic band structures were all examined.

The geometry of small diameter single walled carbon nanotubes significantly differs from that expected from the simple graphene wrapping model. The deviations increase with decreasing diameter (d) and show strong chirality-dependence, this is the hallmark of the individuality of single walled carbon nanotubes.

The radial breathing mode (RBM) frequency shows a significant, *chirality-dependent* deviation from the simple $1/d$ rule which describes the larger diameter tubes well. The RBM is coupled to the totally symmetric tangential modes, and while this coupling is generally small, it is not neglectible. The frequencies of the totally symmetric tangential modes in general follow one of two branches when plotted as a function of tube diameter, with a few exceptions which again are an indication of the strong individuality of small diameter carbon nanotubes.

The behavior of the band gap also shows a significant deviation from the expectation of the zone folding approximation. Enhanced "buckling" is observed for zigzag tubes, showing that the trigonal warping is larger than what is expected from simple tight binding approximation. In the case of zone folding metallic tubes, curvature induces a small secondary gap in the band structure for non-armchair tubes and a downshift of the Fermi wave vector for armchair tubes. Anomalous diameter scaling is found for the secondary gap, which can likely be resolved by considering many-electron effects. In the case of the smallest diameter tubes, the band gap almost always disappears due to $\sigma - \pi$ rehybridization. Some slight chirality-dependence can be observed here, which is another indication of the strong individuality of the small diameter nanotubes.