

Benchmark solutions for REBO potentials

Get ["/mydirectory/Benchmark_code.m"]

show

armchair

zigzag

n

3

radius [nm]: 0.2111

cohesive energy [ev/atom]: -7.0137

Young modulus [GPa]: 890.5525

Poisson coefficient: 0.149

Instructions

1. Load the package "Benchmark_code.m" inserting the directory in "Get" command and press "Shift+Enter"
2. Choose armchair or zigzag CNTs
3. Choose the chiral number n
4. Press Enter to visualize the benchmark results

Note

The code is set for 2nd generation Brenner potential. In order to check another REBO potential, it is necessary to define the proper potential functions and all the corresponding parameters in the "Benchmark_code.m" file.