Doctoral school of Physics - Eötvös Loránd University (ELTE)

First Semester report

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PhD Thesis title: **Modifying and parameterization of Brenner potential and its implementation in molecular dynamics simulation (LAMMPS)**

Introduction

There is a growing interest in the research of chemical reaction inside carbon nanotubes. In other words, the reactions happen in constrained space instead of free space and lead to the growth of new materials. The well-known example is annealing of C_{60} filled by single-walled carbon nanotubes, with diameters of 14 Å, which results in the formation of an inner nanotube. After this, smaller organic molecules such as ferrocene $Fe(C_5)_2$ have been used as filler materials. Followed by the annealing process, in the Raman spectrum there appeared several new bands that seemed initially, an inner carbon nanotube come into existence from the ferrocene molecules. Recently a molecular dynamics simulation with DFT adjusted tight bonding have performed by replacing several numbers of C_5 carbon rings inside a small diameter carbon nanotube. The results have shown interesting carbon structure formation in nano chambers such as carbon chain, ribbons-like and fullerene-like structures, depending on temperature and density [1].

Although they confirm experimental results since the simulation is based on tight binding potential with intensively and time-consuming computation, they cannot be able to implement for large molecules or molecule containing not only carbon atoms (hydrocarbon molecules). Furthermore, the result includes unphysical carbon structures like triangle and square which are clearly unphysical.

Research work

Motivated by above mentioned, it can be a good idea that instead of the tight-binding Hamiltonian we use simply Brenner type potential to describe the interaction between atoms. The Brenner potential is based on Tersoff formalism with additional terms that correct an inherent over-binding of radicals and that include nonlocal effects [2]. Atomization energies for a wide range of hydrocarbon molecules predicted by the potential terms compare well to experimental values. The

Brenner potential function is a short ranged and simple expression and can be quickly evaluated. So it should be very useful for large-scale molecular dynamics simulations for chemical reaction.

In the first step we should modify and parameterize the Brenner function as a fitting function for C_2 and C_3 data, obtained from the tight-binding method.

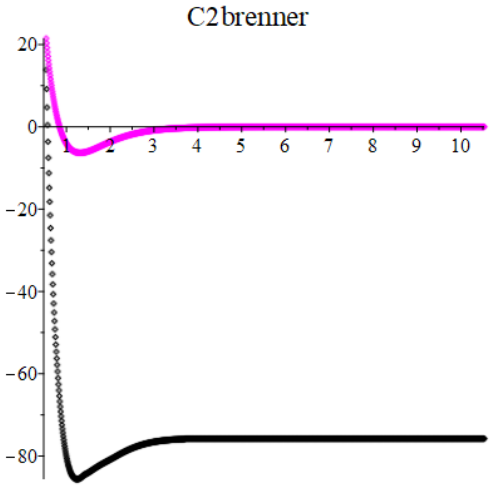

Fig 1. The difference between Brenner (red) and tight-binding (black) data

Studies in current semester

Atomic and Molecular Physics (atmolphysf17vm)

As my work is related to the molecular dynamics and I didn't attend this course in my master degree program, it was the main course in this semester. I learned about some approximation methods applied for atomic and molecular orbitals calculations. Furthermore, I learned how to use Hund's rules, atomic configuration and symmetries to determine the energy levels of molecules.

Computational Studies of Electron Systems (cmcompsf17em)

The goal of this course was to be familiar with computational code of SIESTA based on the Density Functional Theory (DFT). My project was the investigation of the electronic properties of double walled carbon nanotubes. To do this, I wrote an input file in fdf format. Then the code executed to plot the band structure and DOS associated with my DWCNT structure.

References

[1] István László, Bálint Gyimesi, János Koltai and Jenő Kürti, Molecular Dynamics Simulation of Carbon Structures Inside Small Diameter Carbon Nanotubes, Phys. Status Solidi B 2017 1700206

[2] Donald W. Berenner, Empirical potential for hydrocarbons for use in simulating the chemical vapor deposition of diamond films, Phys. Rev. B, **42 (15)**, 9458-9471, 1990