Classical Molecular Dynamics simulations for carbon-based materials

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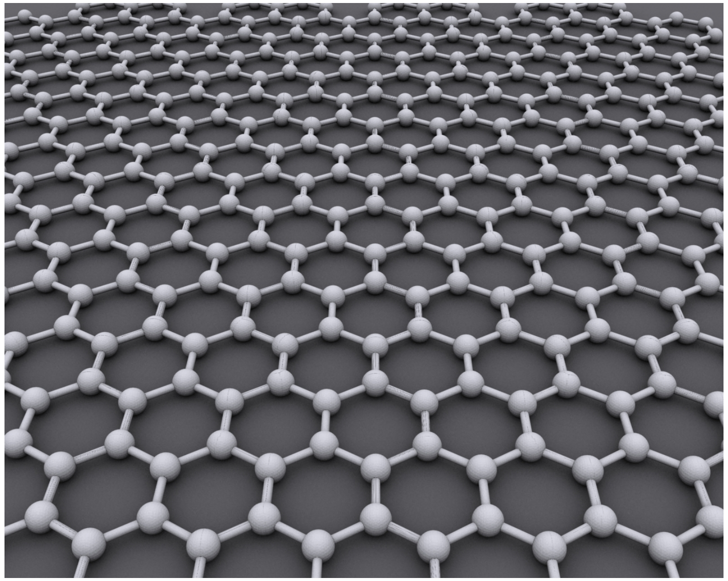
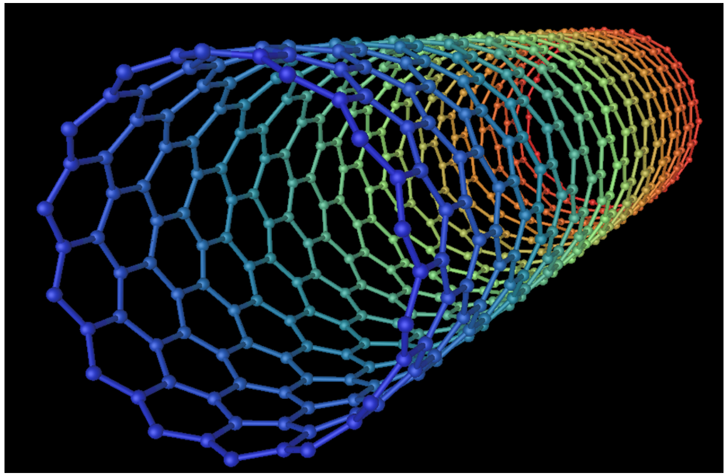
Introduction

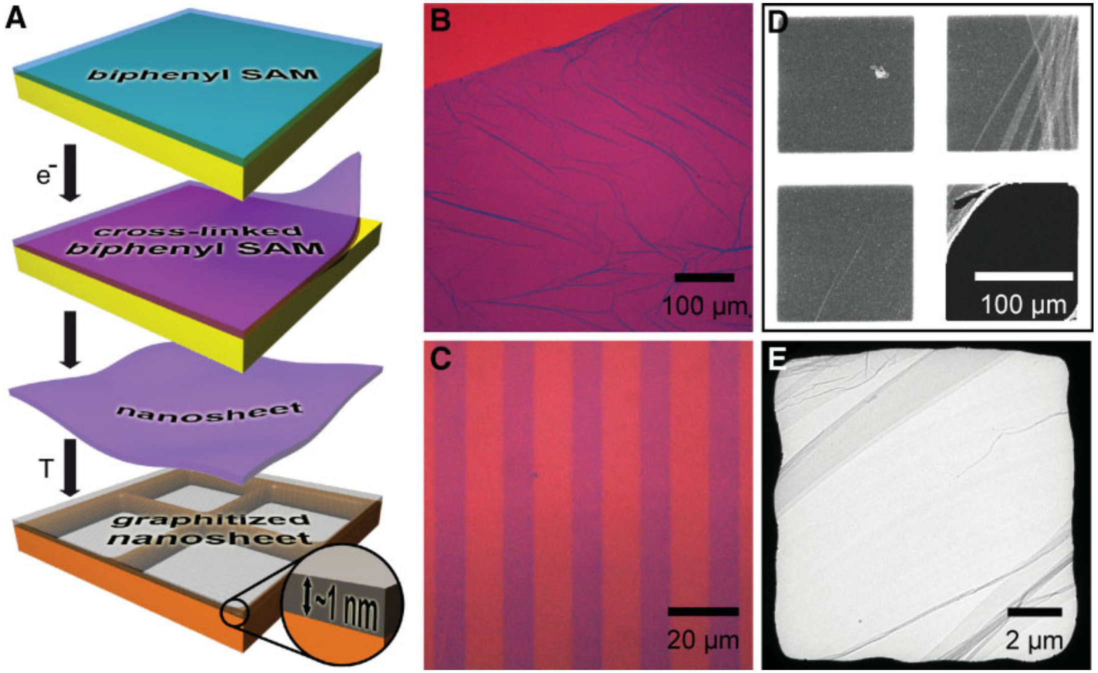
There are various carbon-based nanostructures . . .

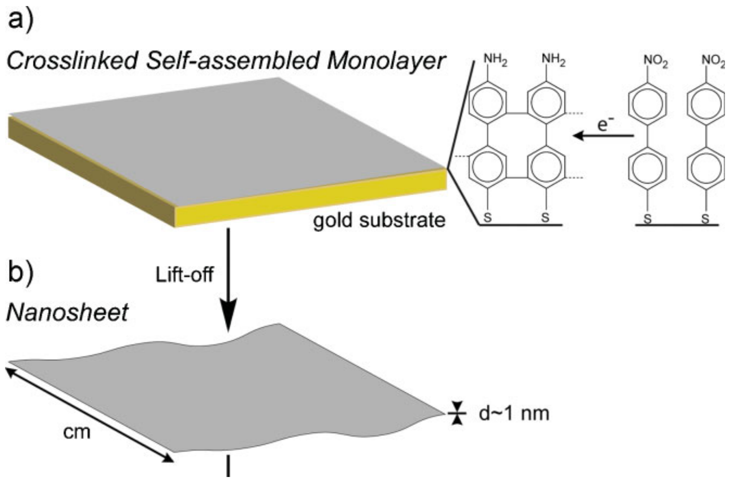




. . . and carbon-based cross-linked SAMs.

ADVANCED MATERIALS





A. Turchanin *et al.*, Advanced Materials **21**, 1233 (2009); I. Amin *et al.*, Small **6**, 1623 (2010).

Problems

- Systems contain very many carbon atoms.
- Structure might be irregular. Defects?
- Quantum Methods, even DFT, cannot deal with such systems.

Thank God, we have computers

“Espresso-doped multi-core”

128 cores, 384 GB RAM

. . . but that’s not enough!

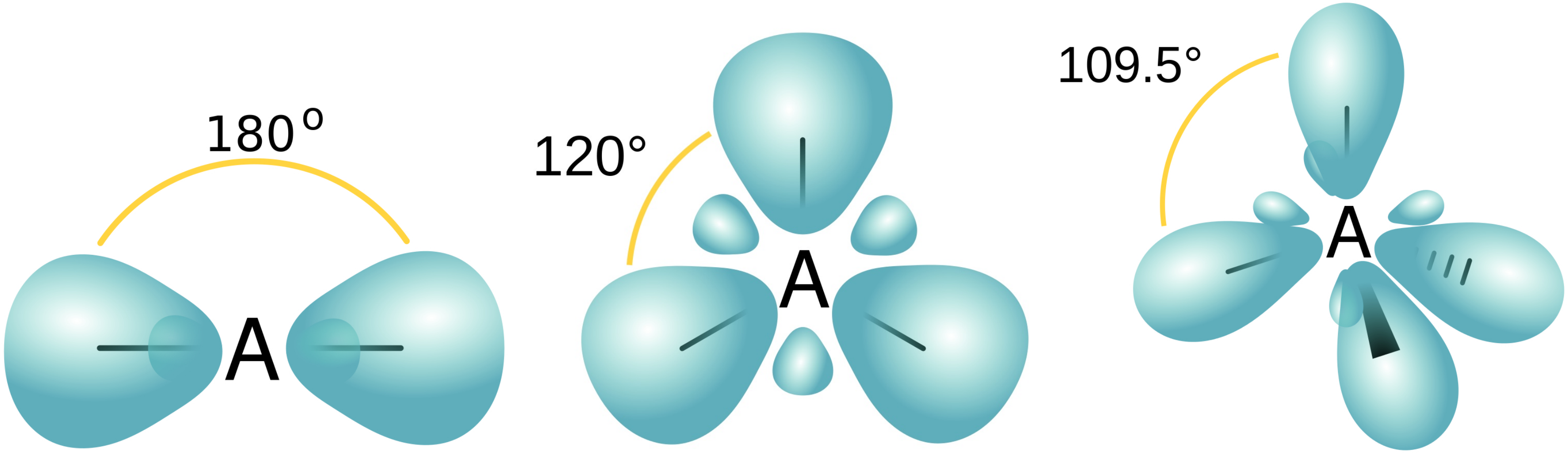
Classical Molecular Dynamics

H. Feldmeier and J. Schnack, Rev. Mod. Phys. **72**, 655 (2000).

Classical Molecular Dynamics

- CMD can model very large systems (∼ $10.000.000$ particles).
- CMD can find ground states and model dynamics.
- But how should this be realistic for carbon-based compounds, where the chemical bond is of quantum nature?

sp hybridization modes



sp, sp^2, and sp^3 hybridization modes.

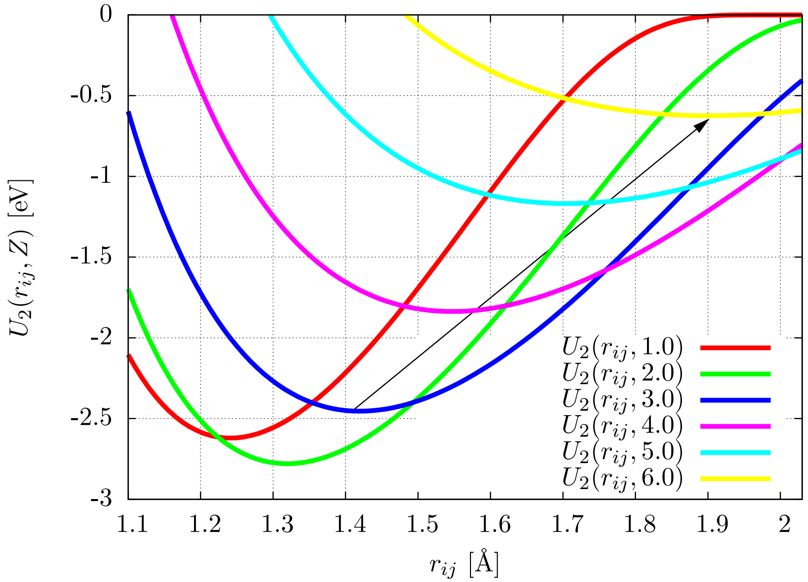
wikipedia: orbital hybridization

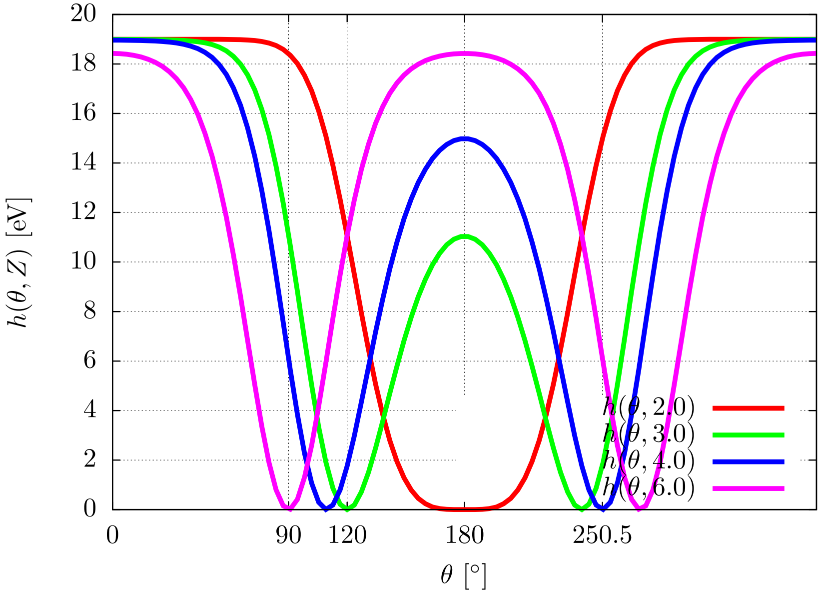
Very sophisticated carbon potential

$$
\begin{aligned}
H(\vec{r}_1, \vec{p}_1; \vec{r}_2, \vec{p}_2; \dots) &= \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + V(\vec{r}_1, \vec{r}_2, \dots) \\
V(\vec{r}_1, \vec{r}_2, \dots) &= \sum_{i \neq j}^{N} U_2(|\vec{r}_i - \vec{r}_j|, Z_i) + \sum_{i \neq (j<k)}^{N} U_3(|\vec{r}_i - \vec{r}_j|, |\vec{r}_i - \vec{r}_k|, \Theta_{ijk}, Z_i)
\end{aligned}
$$

D. W. Brenner *et al.*, J. Phys.: Cond. Mat. **14**, 783 (2002).
N. A. Marks, Phys. Rev. B **63**, 035401 (2000).

Coordination dependence





Coordination influences strength and direction of bonding.

N. A. Marks, Phys. Rev. B **63**, 035401 (2000).
A. Mrugalla, Master thesis (2013), in preparation.

What can be achieved realistically?

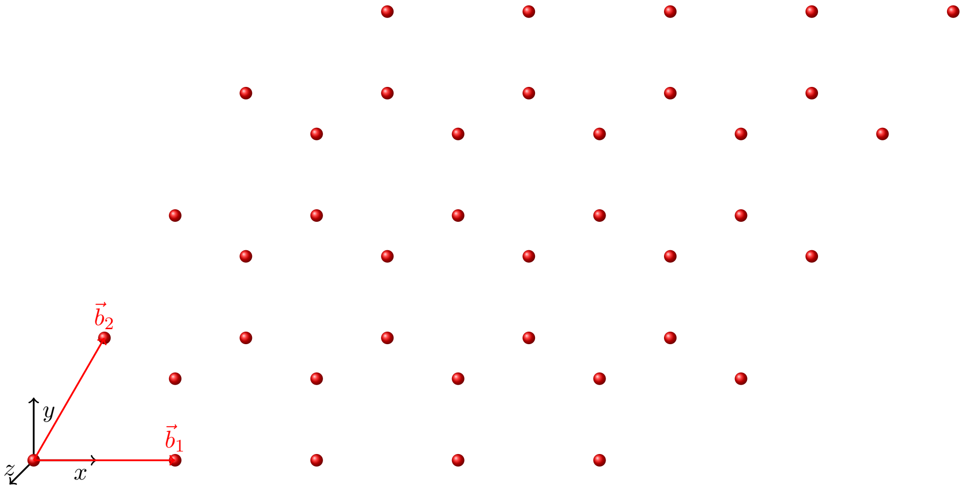
- Structure calculations.
- Dynamical self-organization (1).
- Mechanical properties, such as vibrational spectra and response to mechanical stress.
- Sorry, no electronic properties, such as conductance or heat conductance.

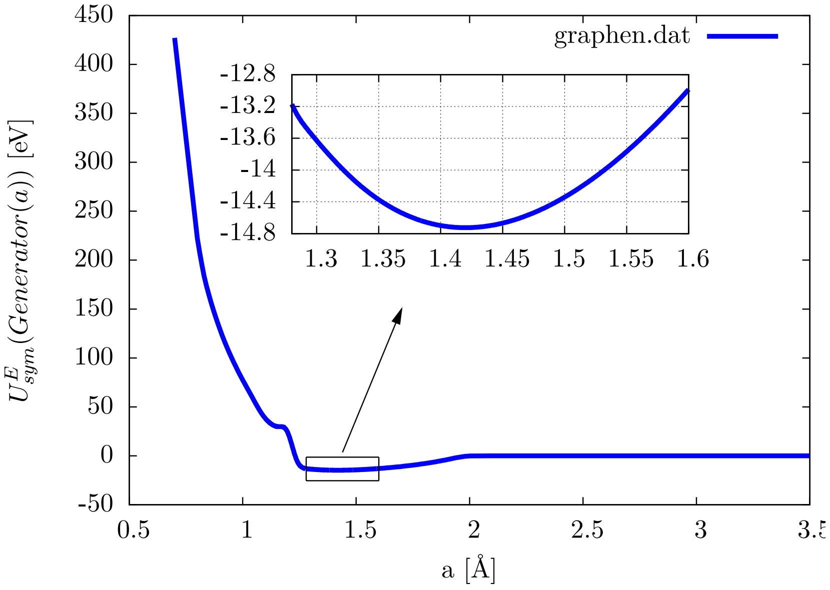
(1) R. C. Powles, N. A. Marks, and D. W. M. Lau, Phys. Rev. B **79**, 075430 (2009).

First investigations

A. Mrugalla, Master thesis (2013), in preparation.

Graphen

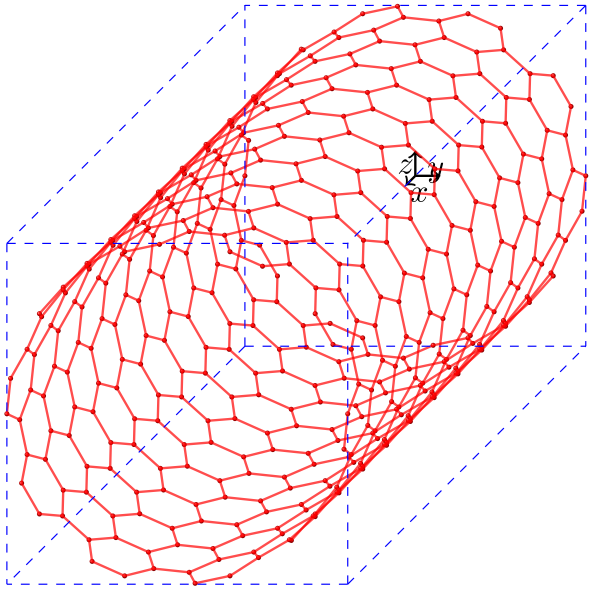


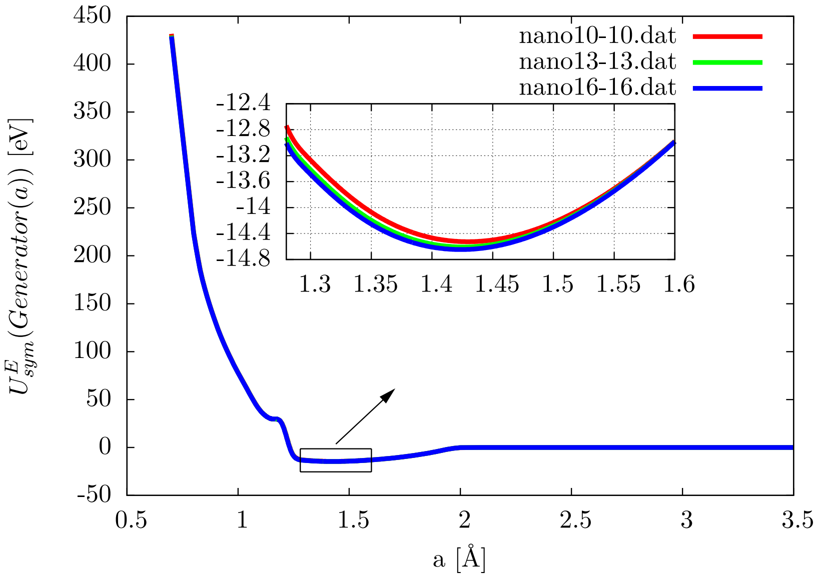


Carbon-carbon distance $a = 1.42$ Å as in reality.

A. Mrugalla, Master thesis (2013), in preparation.

Nanotubes

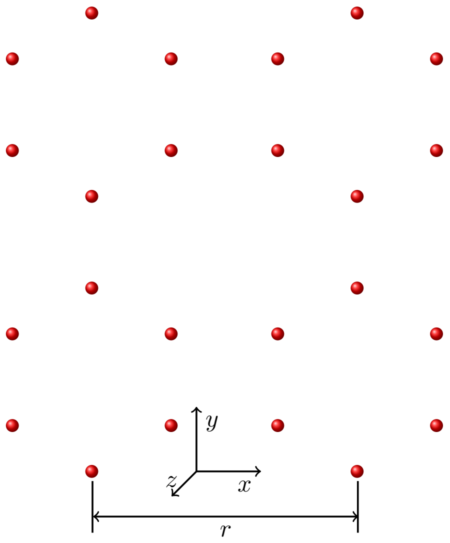


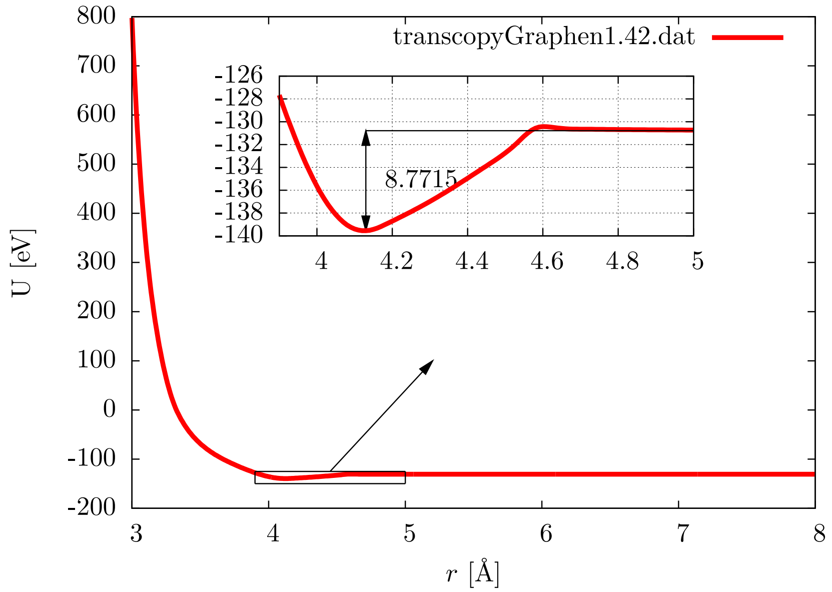


Lattice constant depends slightly on tube structure.

A. Mrugalla, Master thesis (2013), in preparation.

Biphenyl



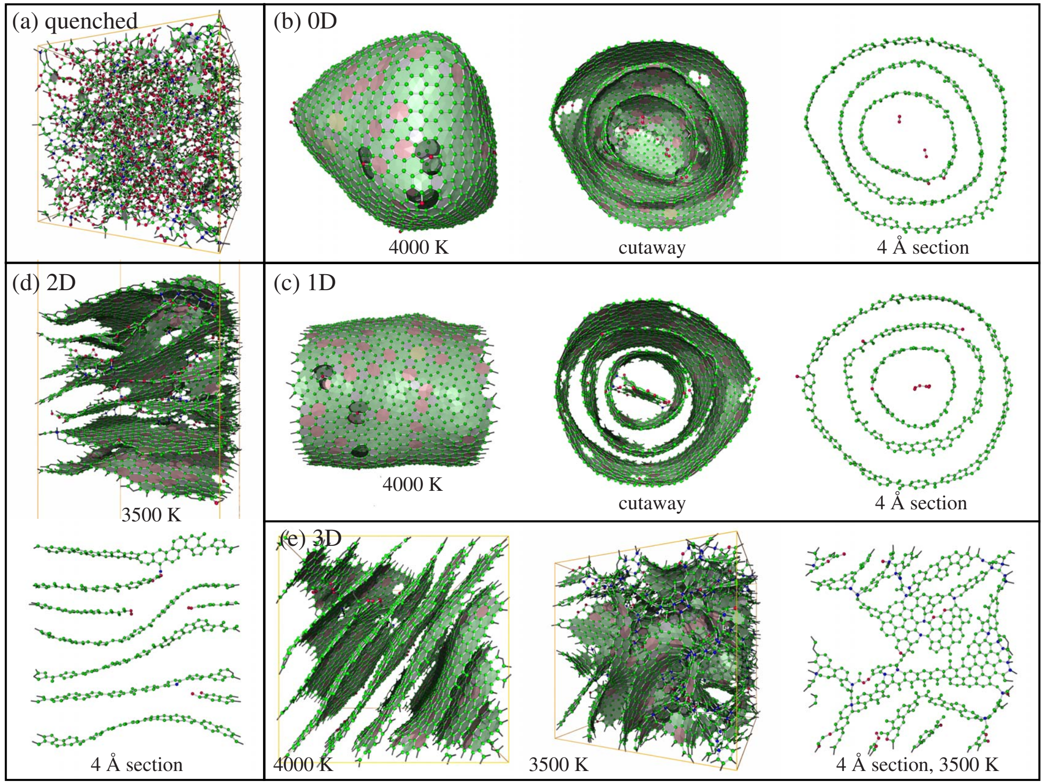


Biphenyls are attractive with a preferred distance of $r \approx 4.1$ Å.

A. Mrugalla, Master thesis (2013), in preparation.

Outlook

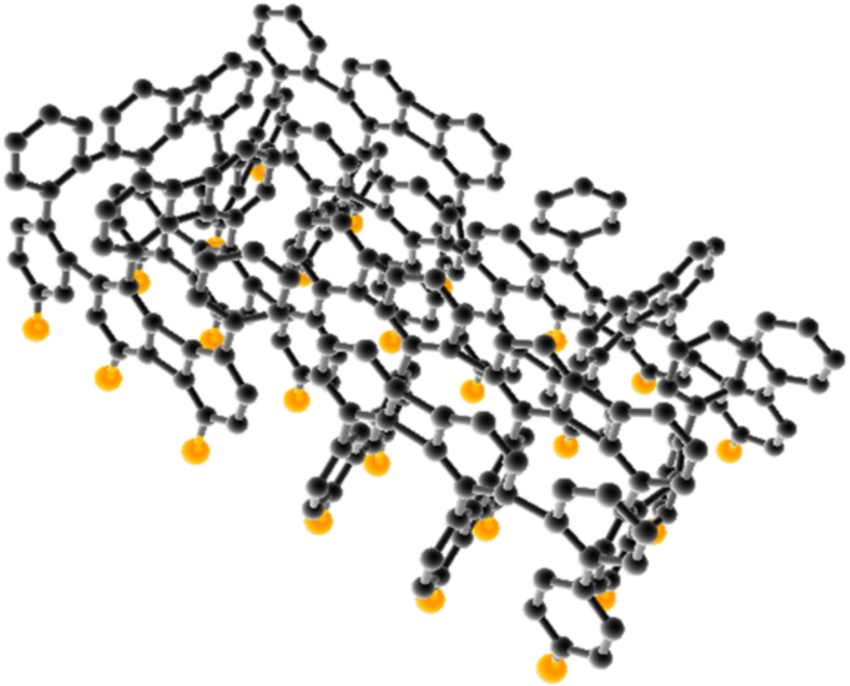
Outlook



Self-organization and sp^2 ordering in large systems.

R. C. Powles, N. A. Marks, and D. W. M. Lau, Phys. Rev. B **79**, 075430 (2009).

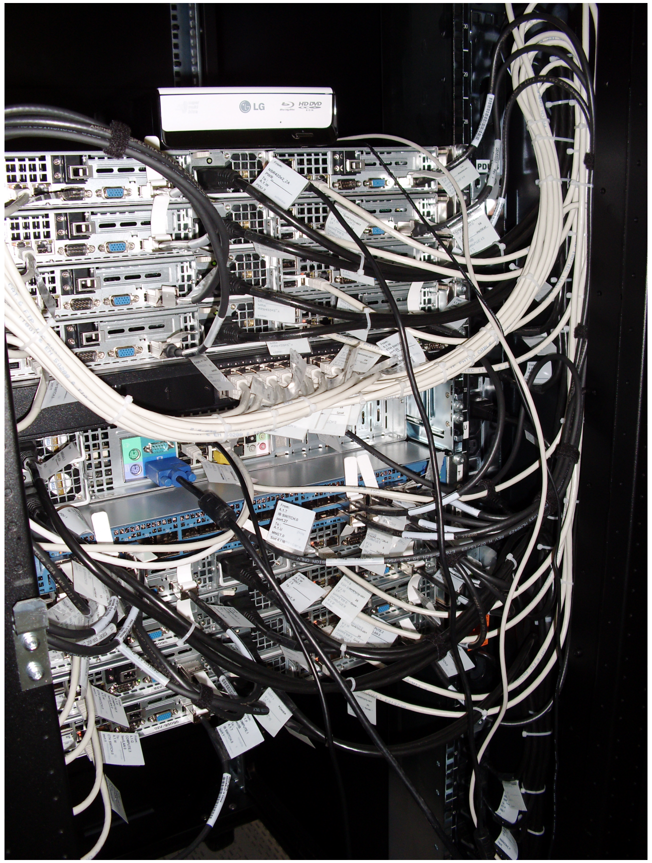
Outlook



Possible real configuration of a Biphenyl layer (1).

(1) D. Rhinow, N.-E. Weber, A. Turchanin, J. Phys. Chem. C **116**, 12295 (2012).

Summary



- Classical Molecular Dynamics can be set up for carbon systems using effective many-body carbon potentials.
- Ground-state geometries can be determined with great accuracy (exception graphite).
- Dynamical self-assembly can be simulated.
- Prospect to simulate nano sheets with realistic, i.e. probably irregular structure.
- Electronic properties CANNOT be modeled.

Many thanks to

Professor Nigel Marks, Curtin University, Australia

Thank you very much for your attention.