Advanced modeling techniques: Particle-swarm optimization

Parthapratim Biswas

The University of Southern Mississippi

OUTLINE

- An overview of inverse/hybrid approaches
  - Reverse Monte Carlo (RMC) simulations
  - Beyond RMC: Hybrid approaches (ECMR, FEAR, INDIA, etc.)
  - Population-based swarm intelligence
- Optimization of finite systems
  - Lennard-Jones clusters
  - Finnis-Sinclair and Sutton-Chen (Fe/Cu clusters)
- Bulk materials
  - Amorphous graphene
  - Amorphous silicon

Materials design

Amorphous: *without a clearly defined shape or form*

- Where are the atoms/molecules?
- No translational symmetry (solids sans k-space)
- Structural determination
- Atomistic materials design $\equiv$ a constrained optimization program

"If you want to understand function, study structure" -Francis Crick

Reverse Monte Carlo simulations

$$\Xi = \sum_i \left[\frac{S^{\exp}(Q_i) - S(Q_i)}{\sigma_i} \right]^2 + \sum_j \gamma_j f_j^{c}(X)$$

Key idea and some observations

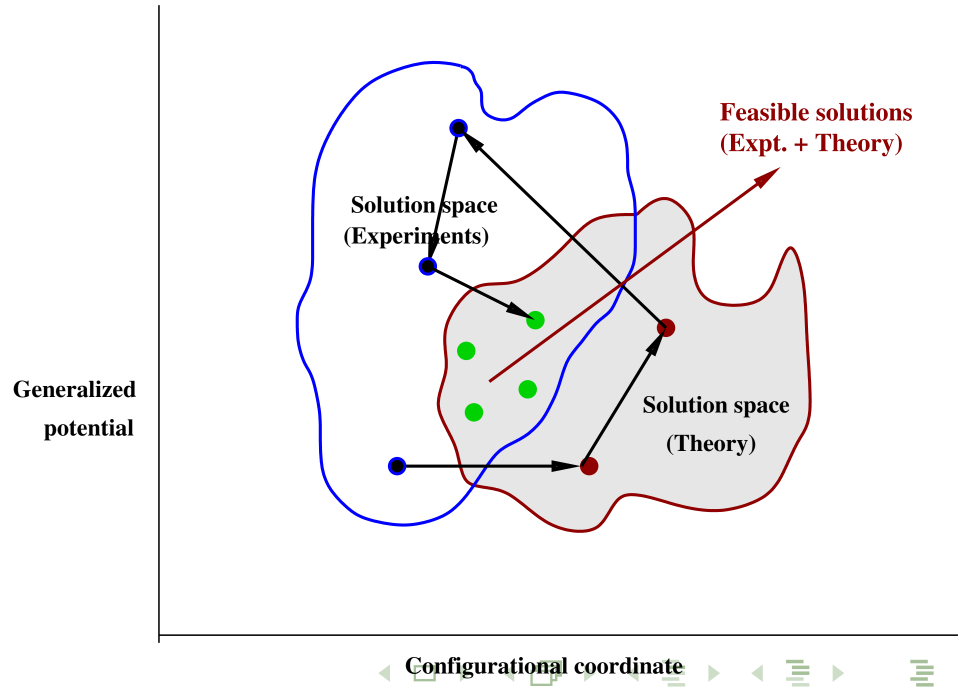
- Inversion of experimental structure factors or pair-correlation data
- Use few constraints to include additional (e.g. topological) information
- Avoid too many competing constraints (pareto-optimality)
- Difficult to produce *necessary* higher-order correlations functions (beyond pair correlations).

McGreevy, R. L. JPCM 2001
Biswas + Atta-Fynn + Drabold, PRB 2004

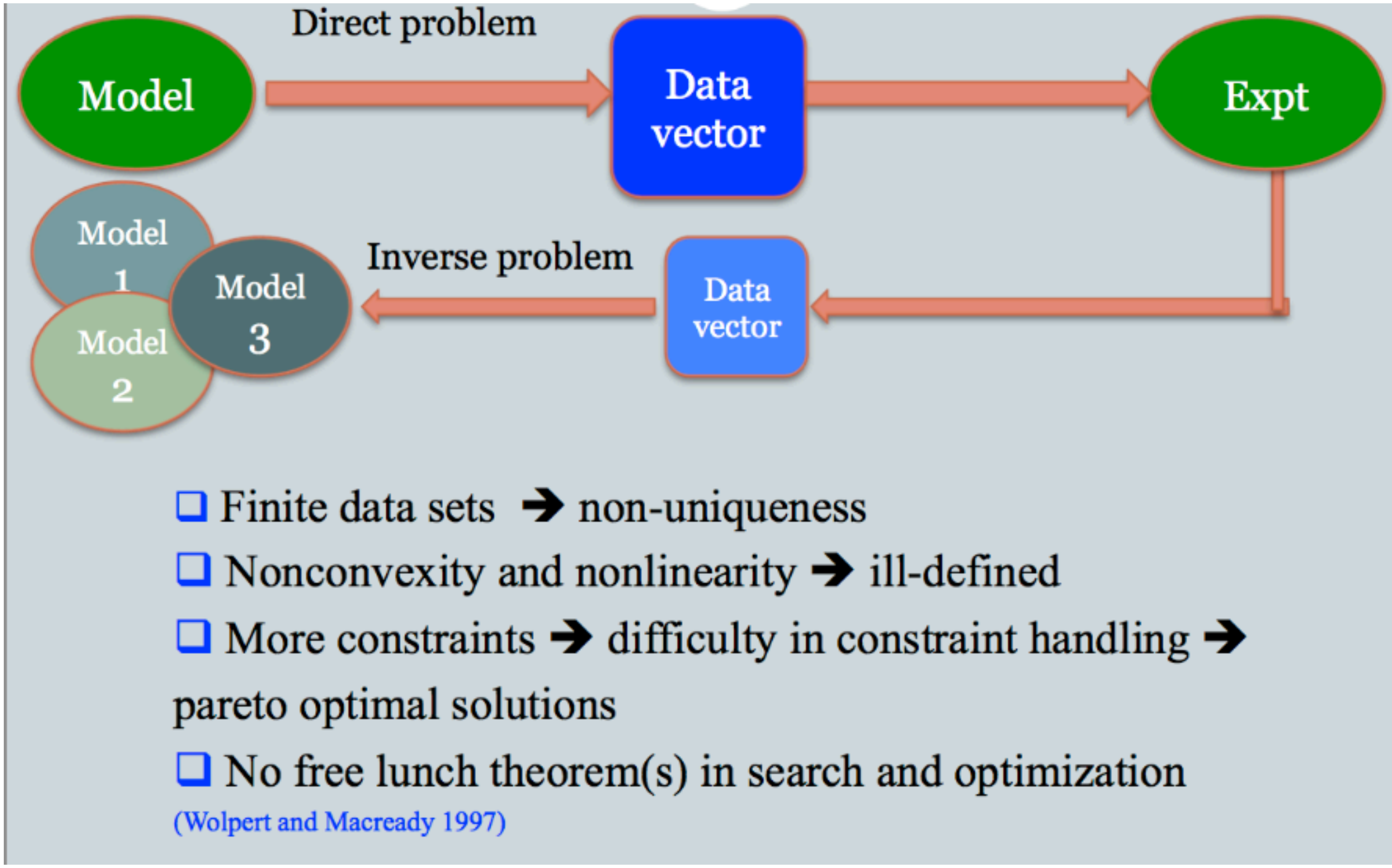
Hybrid approaches: Merging theory with experiments

- 'Melt-quench' MD: highly successful but has limitations (e.g. *a*-Si, *a*-Ge, etc).
- Hybrid philosophy: combine experimental data with simulations – form an *augmented* solution space
- Choose from *experimentally-feasible* solutions – obtain self-consistency between force-fields and experimental data. Several schemes are possible, e.g., ECMR, FEAR, INDIA

Biswas + Tafen + Drabold, PRB 2005
Biswas + Atta-Fynn + Drabold, PRB 2007
Atta-Fynn + Biswas, JPCM 2009
Pandey + Biswas + Drabold, PRB 2015
Prasai + Biswas + Drabold, Sci. Rep 2015

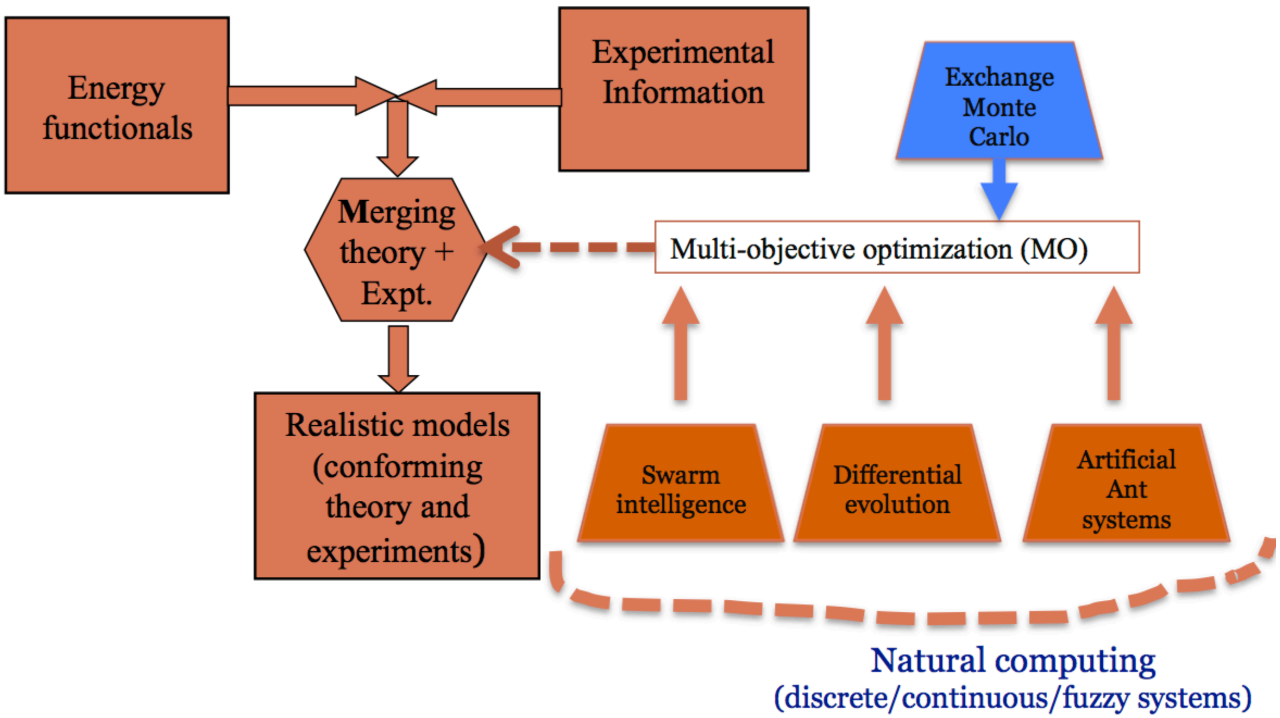


Inverse/hybrid approaches: curse of high dimensionality



Observation: Glass-structure determination is a difficult optimization problem, associated with computational complexity theory.

Is P = NP? (a Clay Institute millennium problem; Status: unsolved)



Biswas + Timilsina JPCM 2011
Timilsina + Biswas JPCM 2013
Biswas + Drabold + Atta-Fynn JAP 2014
Biswas + Elliott JPCM 2015
Atta-Fynn + Biswas JCP 2018
Limbu et al. PRB 2018

Particle Swarm Optimization

1. Introduced by Kennedy and Eberhart (IEEE 1995) to understand the social behavior (e.g., graceful but unpredictable 'choreography') of a flock of birds
2. Flock dynamics have a cognitive component and a social component to attain optinal formation
3. Adopted for optmization problems in high dimension

Key ideas

- A population-based stochastic search algorithm
- Motivated by the foraging behavior of a school of fish or a flock of birds
- Mimics socio-psychological behaviors to emulate the success of others!

Implementation

- Swarm size (10–20)
- An ansatz for 'time' evolution
- Ability to simulate socio-psychologcial behaviors
- Knowledge-sharing networks
- A symbiotic cooperative algorithm

Particle Swarm Optimization

1. Introduced by Kennedy and Eberhart (IEEE 1995) to understand the social behavior (e.g., graceful but unpredictable 'choreography') of a flock of birds
2. Flock dynamics have a cognitive component and a social component to attain optinal formation
3. Adopted for optmization problems in high dimension

Key ideas

- A population-based stochastic search algorithm
- Motivated by the foraging behavior of a school of fish or a flock of birds
- Mimics socio-psychological behaviors to emulate the success of others!

Implementation

- Swarm size (10–20)
- An ansatz for 'time' evolution
- Ability to simulate socio-psychologcial behaviors
- Knowledge-sharing networks
- A symbiotic cooperative algorithm

Particles $\equiv$ Bees (with mobile phones!)

Particle Swarm Optimization

1. Introduced by Kennedy and Eberhart (IEEE 1995) to understand the social behavior (e.g., graceful but unpredictable 'choreography') of a flock of birds
2. Flock dynamics have a cognitive component and a social component to attain optinal formation
3. Adopted for optmization problems in high dimension

Key ideas

- A population-based stochastic search algorithm
- Motivated by the foraging behavior of a school of fish or a flock of birds
- Mimics socio-psychological behaviors to emulate the success of others!

Implementation

- Swarm size (10–20)
- An ansatz for 'time' evolution
- Ability to simulate socio-psychologcial behaviors
- Knowledge-sharing networks
- A symbiotic cooperative algorithm

Particles $\equiv$ Bees (with mobile phones!)

Bees bring nectar, pollen, and information to their hives (Von Frisch 1927)

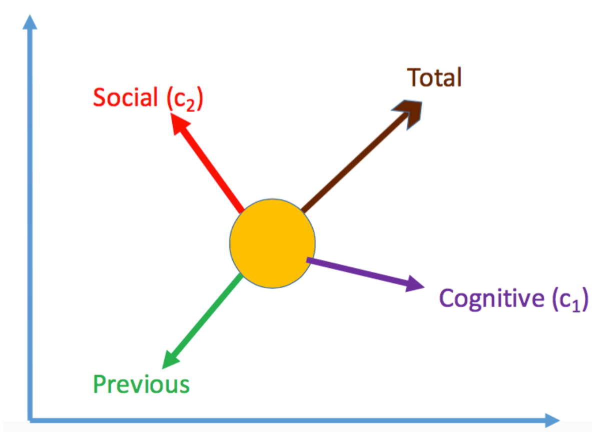
Particle Swarm Optimization

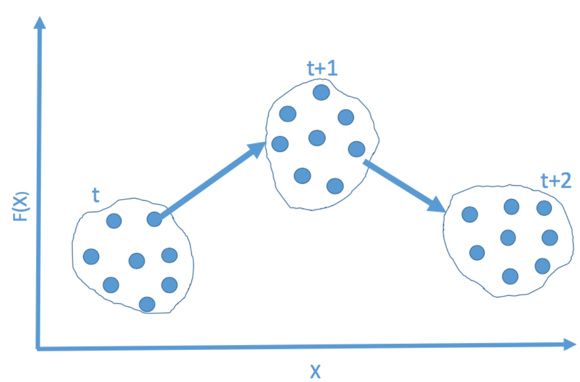
A basic algorithm

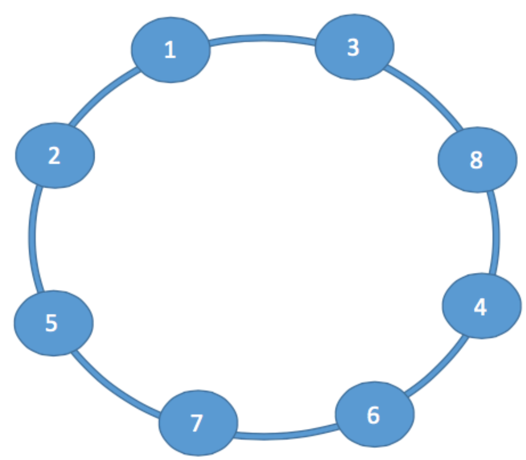
$$
\begin{aligned}
\mathbf{x}_{i+1}(t) &= \mathbf{x}_i(t) + \mathbf{v}_i(t+1) \\
v_{ij}(t+1) &= v_{ij}(t) + c_1 r_{1j}(t)[y_{ij}^{pbest}(t) - x_{ij}(t)] + c_2 r_{2j}(t)[y_{ij}^{gbest}(t) - x_{ij}(t)]
\end{aligned}
$$

$i =$ particle index, $\quad j =$ dimenion

y^{pbest} cognitive component (personal best)
$y^{g/lbest}$ social component (global/local best)
$r_i \in U(0,1)$ $\quad c_1$ and c_2 PSO parameters







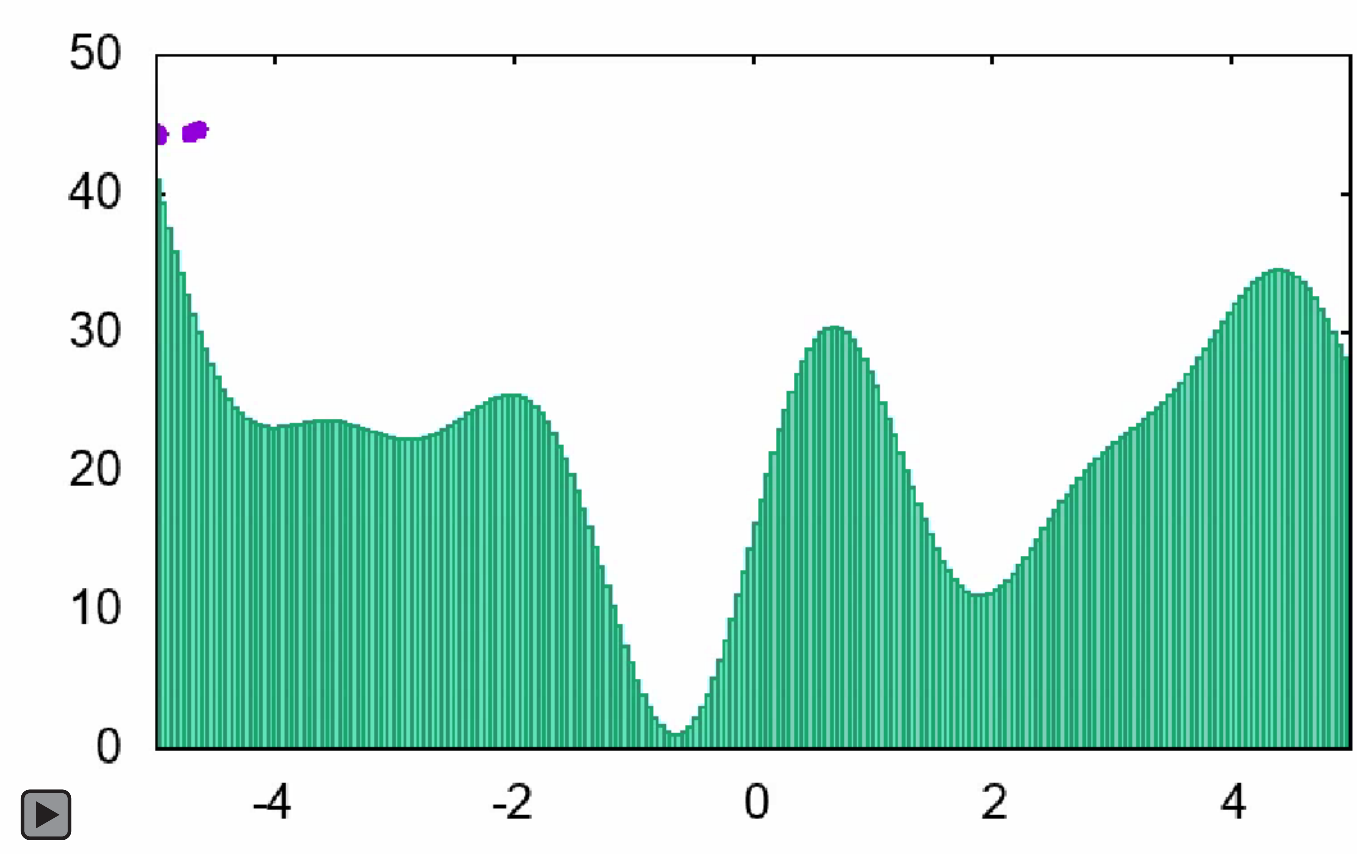
Ring topology for knowledge sharing

PSO: A simple algorithm

Global-best PSO

Create a population "solutions" of size n_p of dimension n_d
repeat
for each particle $i = 1, ..., n_p$
do:
// find personal best
if $(f(x_i) < f(y_i))$ then
$y_i = x_i$
end
// find global best (among all personal best)
if $(f(y_i) < f(y^{gbest})$ then
$y^{gbest} = y_i$
end
end do:
for each particle $i = 1, ..., n_p$
do:
update the velocity
update the position
end do
until convergence criteria are met

PSO: A simple illustration



Evolution in a multi-modal potential

PSO: Applications to LJ clusters

A modified PSO algorithm

1. Local best PSO algorithm
2. Star network geometry for knowledge sharing
3. Population size: 6-20
4. No gradient information
5. Local trapping is avoided by adding several modifications (e.g. rotation and translation in hyperspace)

Compare structures with those from the CCD at

http://www-wales.ch.cam.ac.uk/CCD.html

LJ clusters: PSO versus CCD

N	PSO (eV)	CCD (eV)	ΔE
9	-24.113	-24.113	0.0
10	-28.423	-28.423	0.0
20	-77.177	-77.177	0.0
28	-117.822	-117.823	0.001
30	-128.071	-128.286	0.215
38	-173.156	-173.928	0.772 (*)
40	-185.220	-185.249	0.009
50	-244.492	-244.549	0.057
75	-396.117	-397.492	1.375 (*)

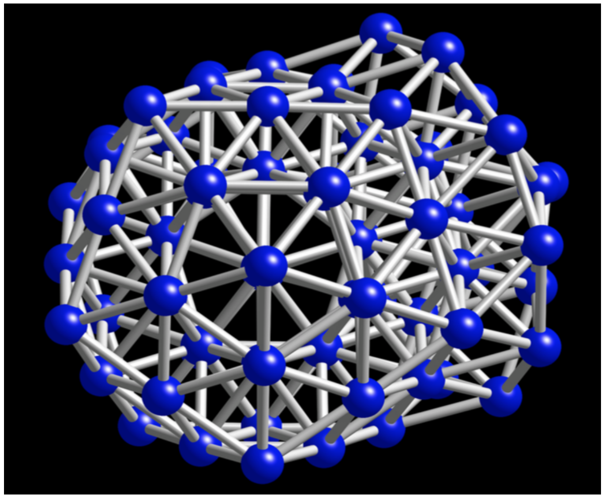
Caution: LJ_{38} and LJ_{75} are the two most difficult cases

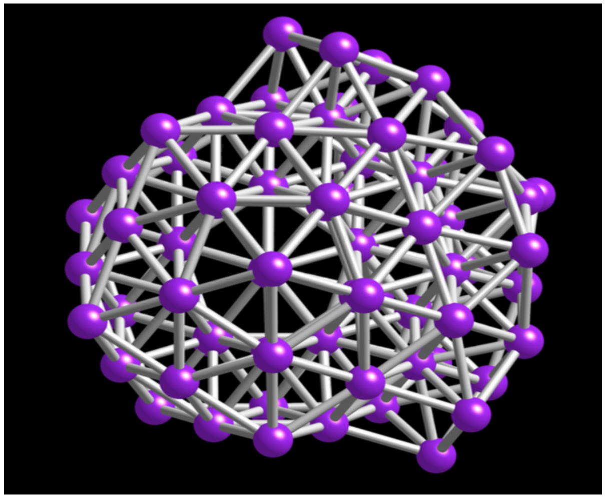
Wales and Doye, J.Phys. Chem. A 1997
Biswas and Elliott 2019 (In prepration)

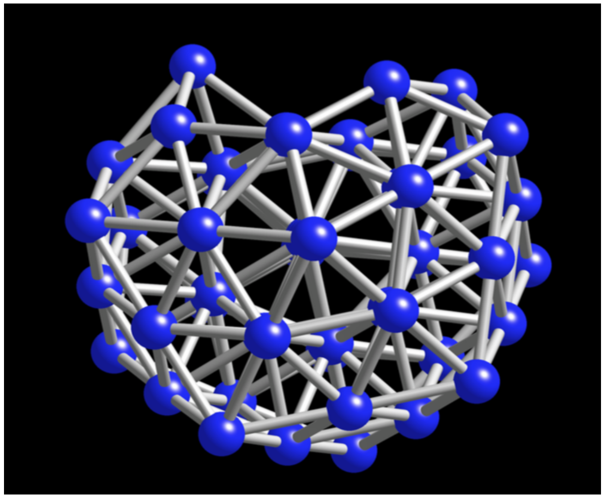
LJ clusters: PSO versus CCD

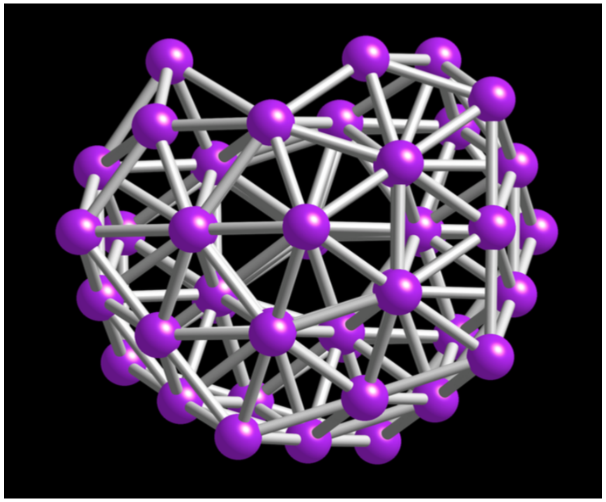
CCD-LJ75 (-396.282 eV)

PSO-LJ75 (-396.117 eV)









CCD-LJ50 (-244.492 eV)

PSO-LJ50 (-244.549 eV)

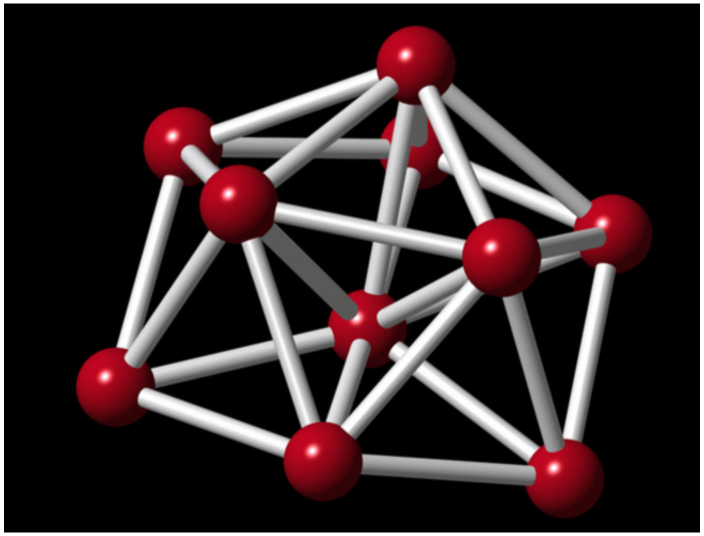
Fe clusters: PSO versus CCD

N	PSO (eV)	CCD (eV)	ΔE
10	-28.535	-28.535	0.0
15	-46.636	-46.637	0.001
20	-64.837	-64.838	0.001
25	-82.938	82.940	0.002
30	-101.448	-101.451	0.003
35	-119.592	-119.597	0.005
55	-194.358	-194.686	0.328

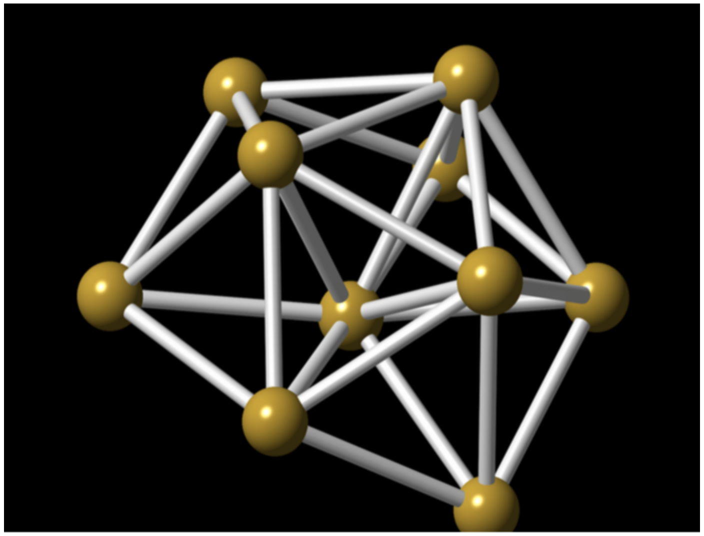
Elliott, Shibuta and Wales, Phil. Mag. 2009

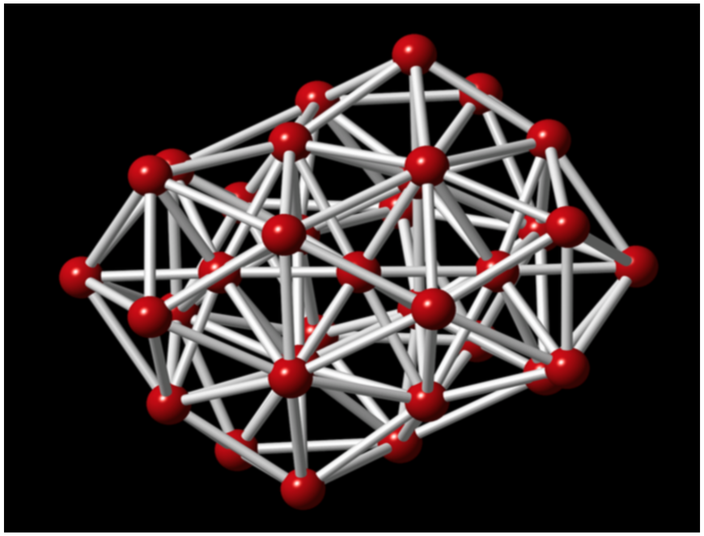
Fe clusters: PSO versus CCD

CCD-FE10 (-28.535 eV)

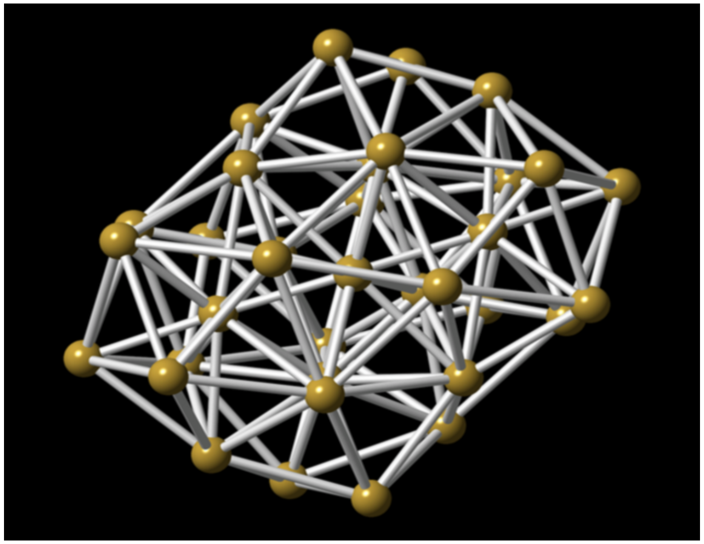


PSO-FE10 (-28.534 eV)





CCD-FE35 (-119.597 eV)

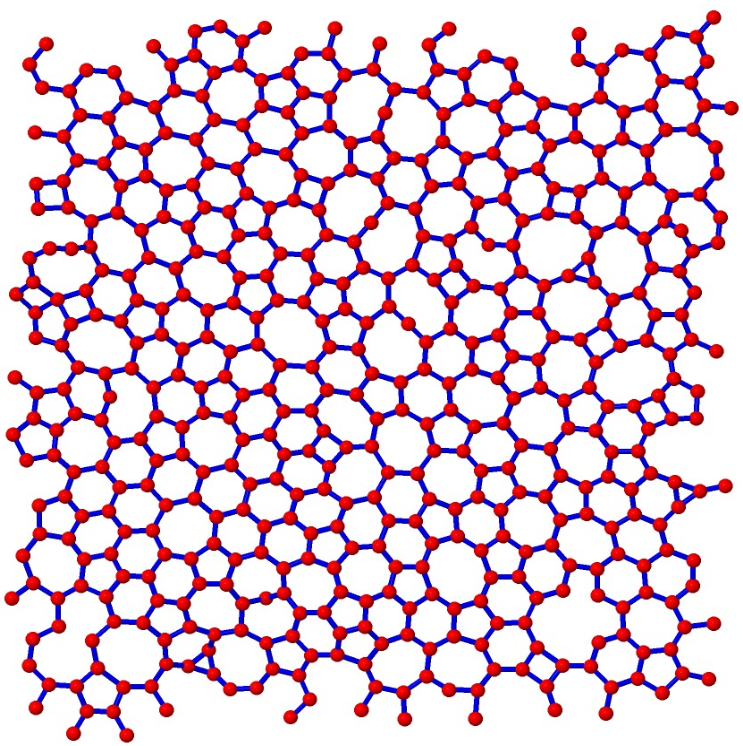


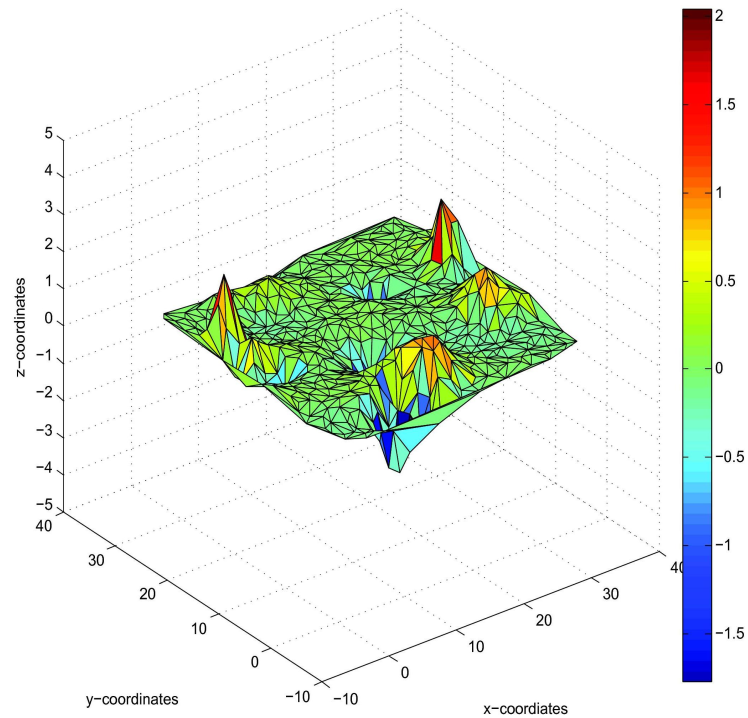
PSO-FE35 (-119.593 eV)

Amorphous or disordered graphene

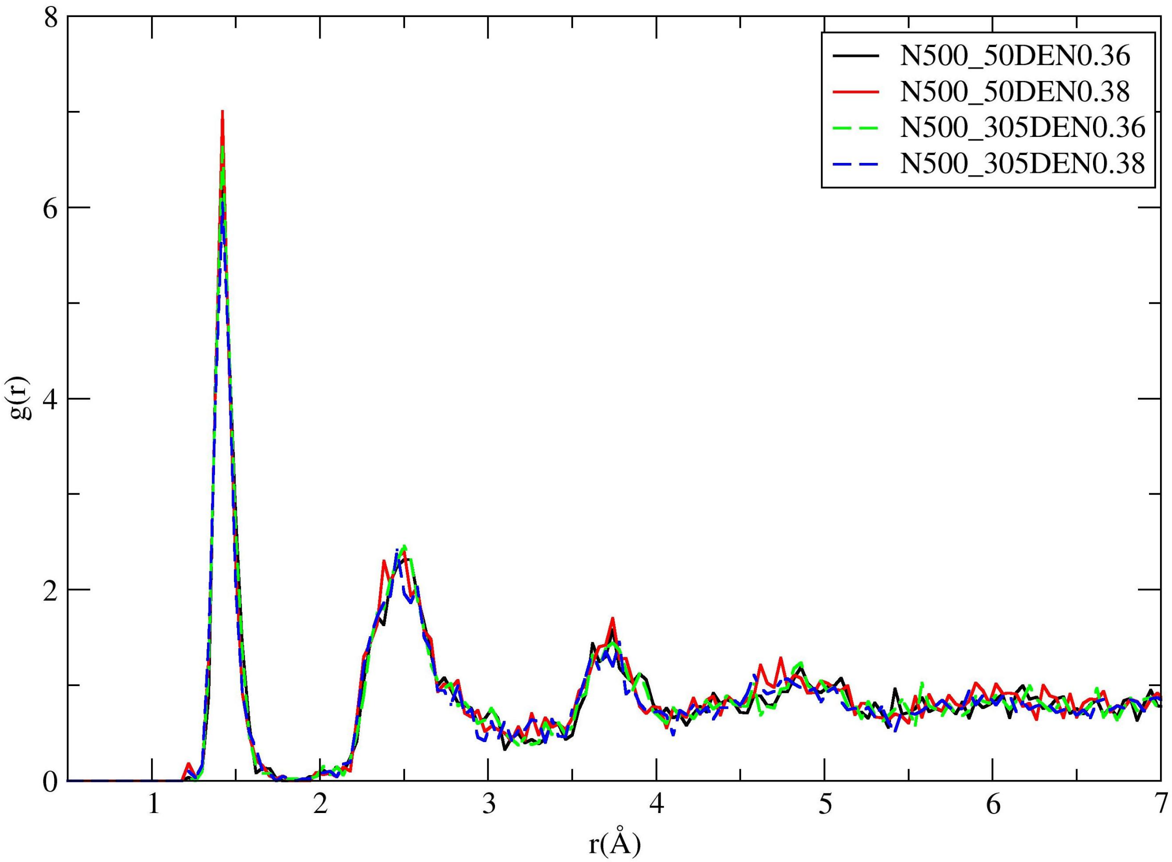
Simulation details

- Size 500 atoms; density 0.36–0.4 atoms/Å^2 (cf. 0.38 for Graphene)
- Bond-order potential followed by *ab initio* relaxations
- Global-best PSO with a swarm size of 8–12

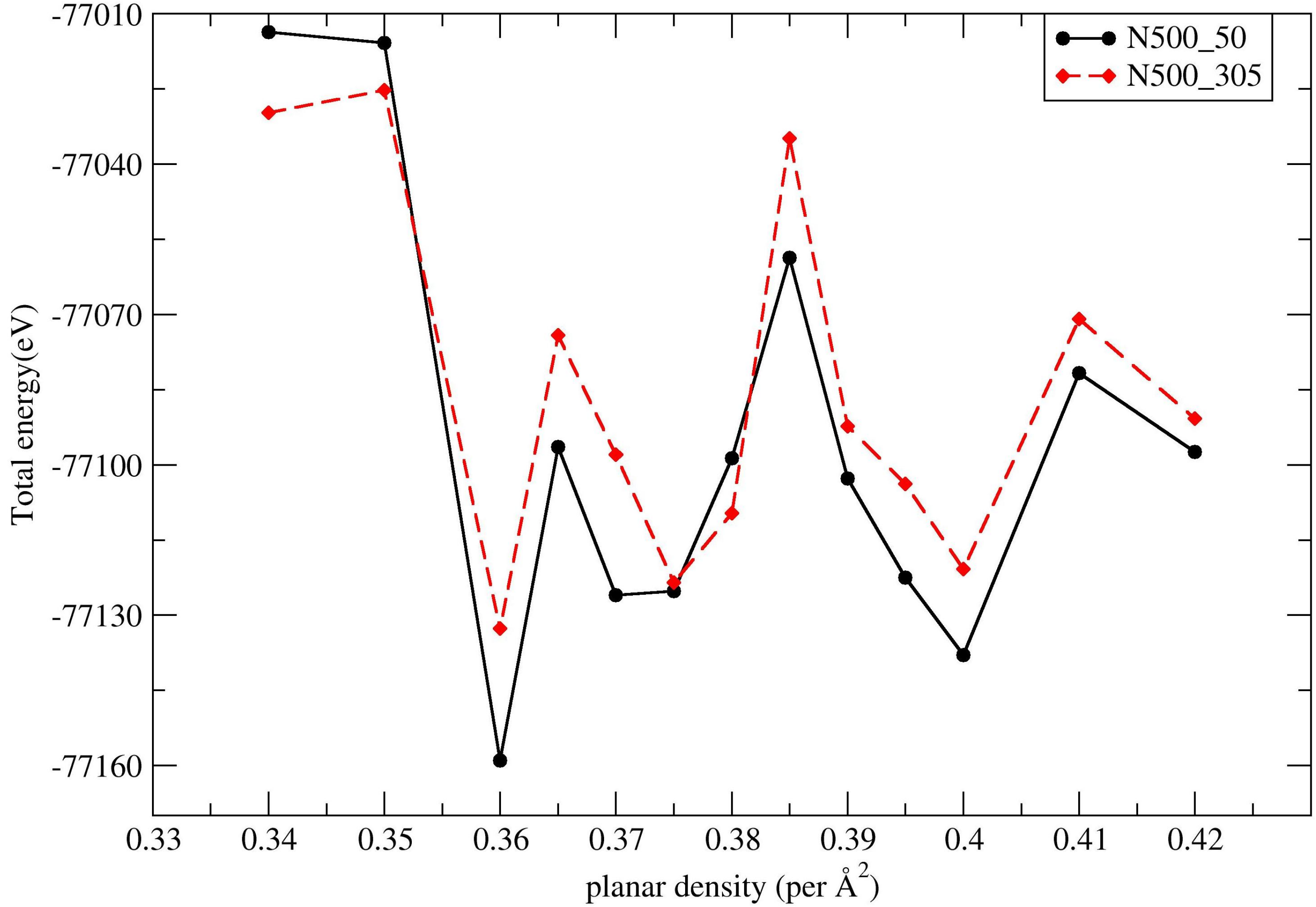




Amorphous graphene: Pair-correlation functions



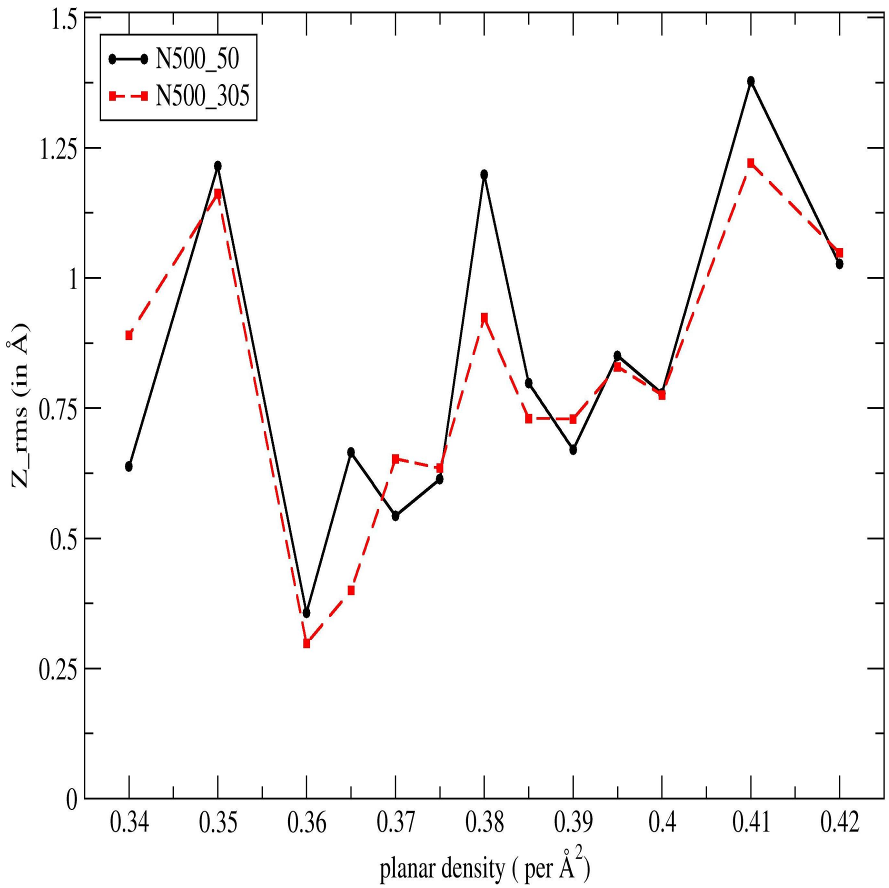
Amorphous graphene: Total-energy vs. planar density



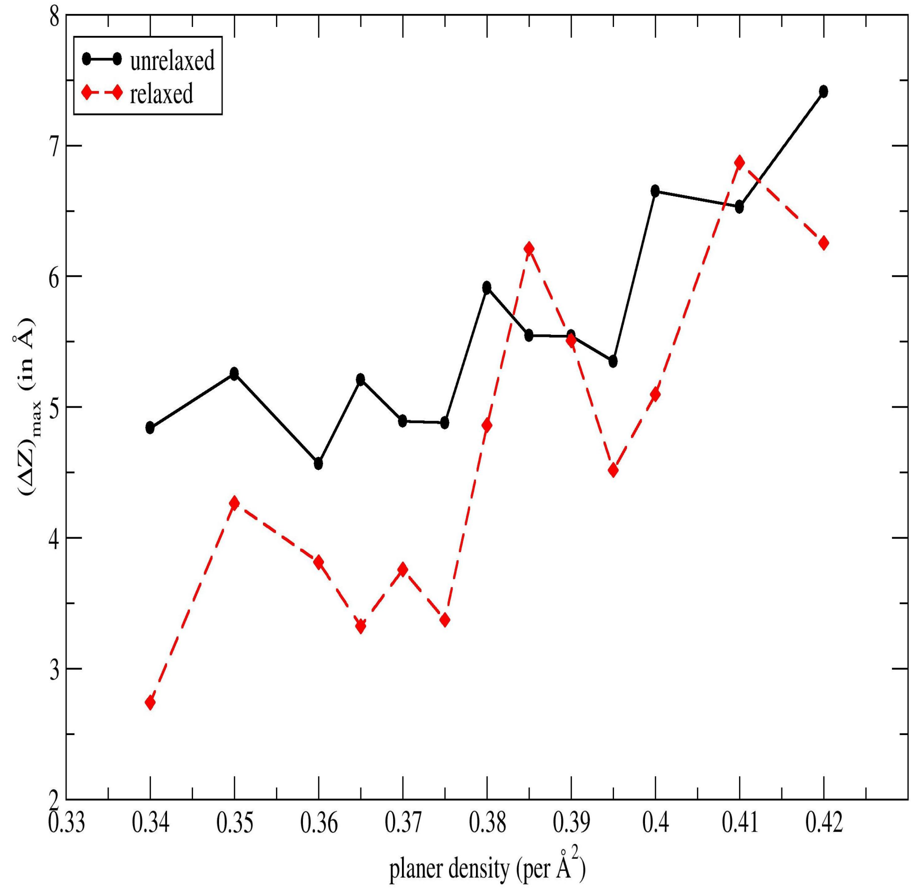
Relaxation: SIESTA with conjugate gradient method

Amorphous graphene: Surface roughness

RMS ΔZ

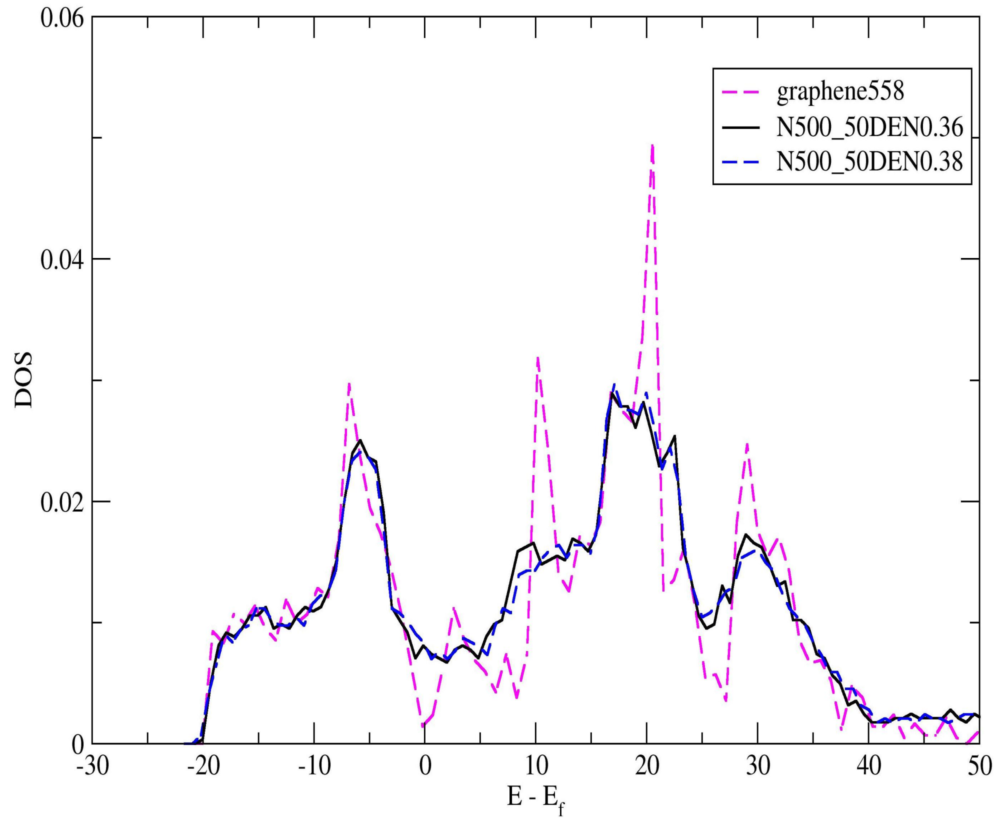


Max ΔZ



Planar density (atoms/Å^2)

Amorphous graphene: Electronic density of states



X axis: E-E_f (in eV); Y axis: DOS (states/eV)

Moot point: metal, semimetal or insulator?

Acknowledgments

- Basudev Oli (Former student, Temple University)
- NSF-Lehigh Materials Research Fellowship (on new functionality of glasses)
- Trinity College, Cambridge (UK)

Thank you!