Simulating the structural diversity of astrophysical carbon clusters

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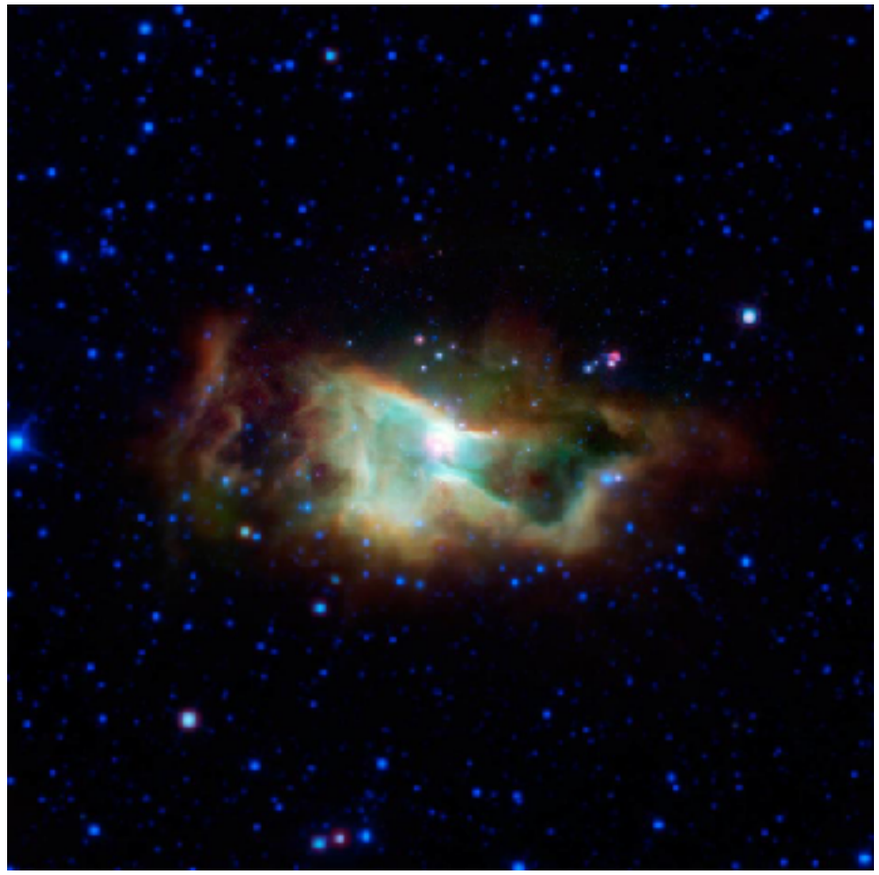
  - Maëlle Bonnin
  - Pascal Parneix
  - Thomas Pino

- Laboratoire Interdisciplinaire de Physique — Université Grenoble Alpes
  - Florent Calvo

Carbon clusters: an astrophysical issue

- ~200 molecules have been detected in the Interstellar medium (ISM)

Horsehead nebula

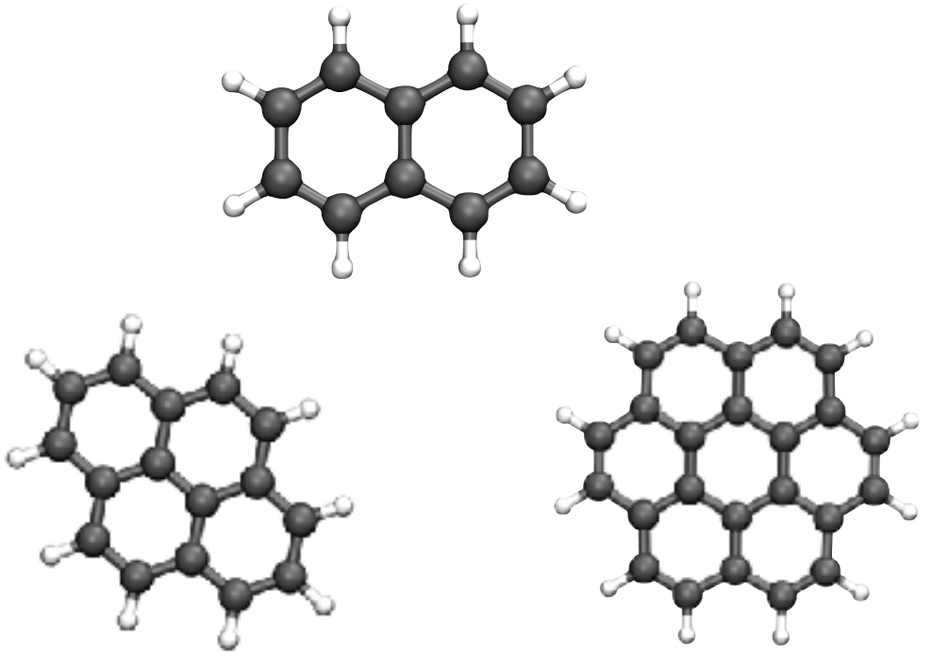


Iris nebula

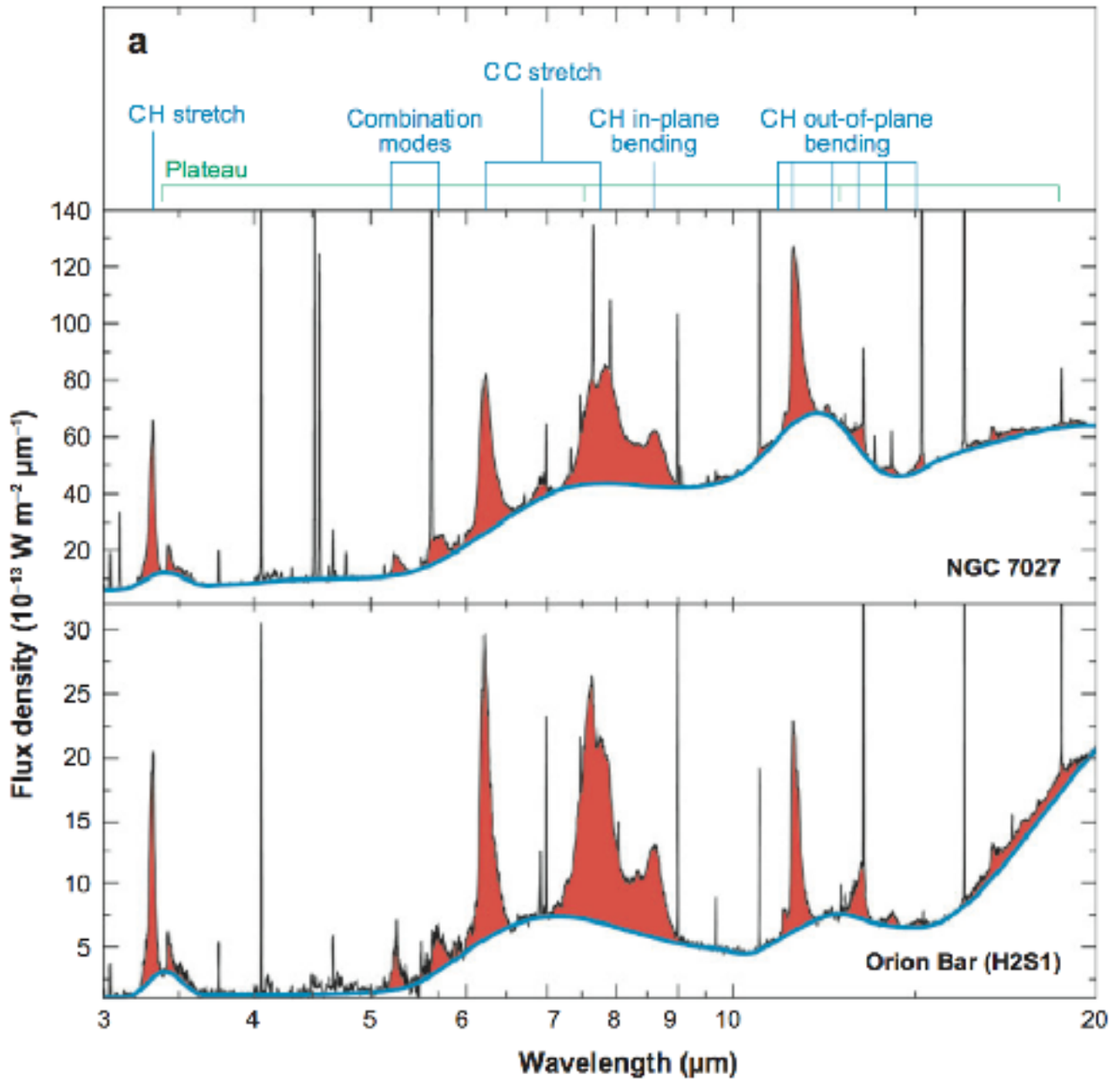
- The ISM is composed of H, He, C, O, N, …

Carbon clusters: an astrophysical issue

- The presence of polycyclic aromatic hydrocarbons (PAH) in the ISM have been suggested for more than 30 years.
- No clear identification of a specific PAH have been achieved



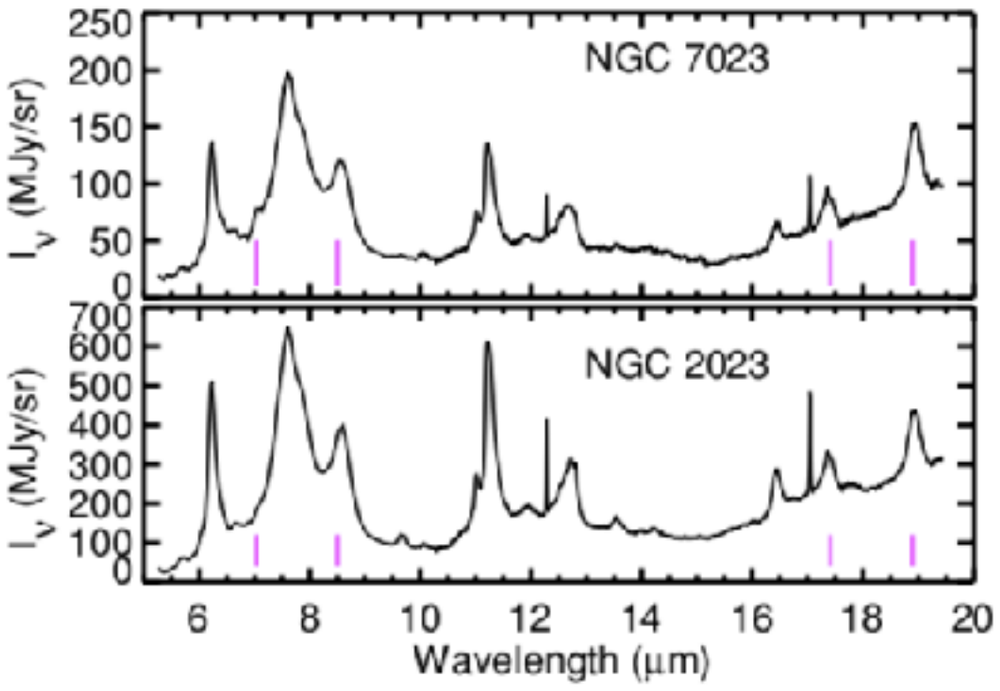
Tielens, Annu. Rev. Astron. Astrophys. 46, 289 (2008)

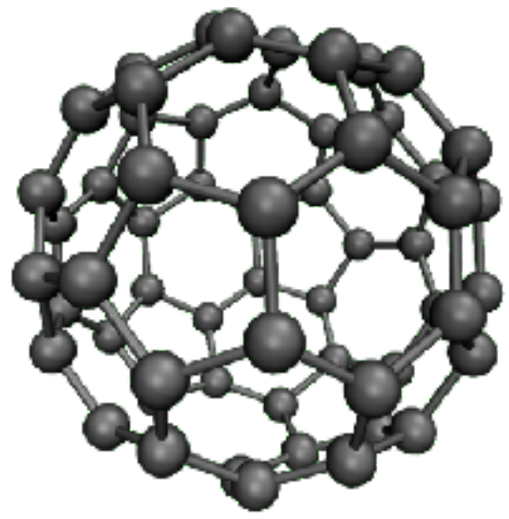


LAMMPS

Carbon clusters: an astrophysical issue

- C_{60} Buckminsterfullerene have been identified in 2010 in the ISM





Sellgren et al. Astrophys. J. Lett. 722, L54 (2010)

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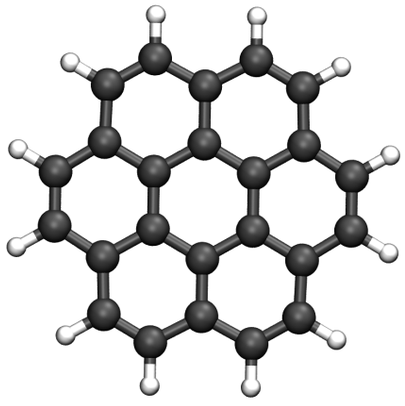
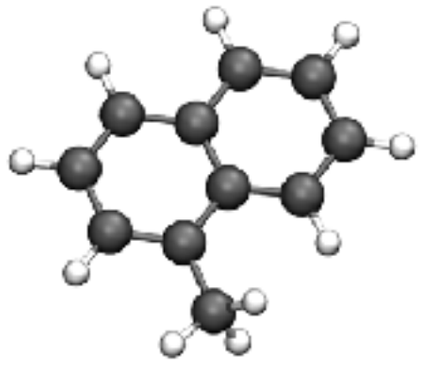
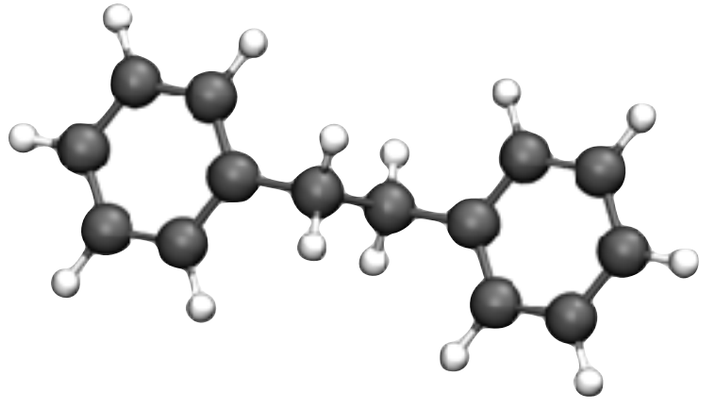
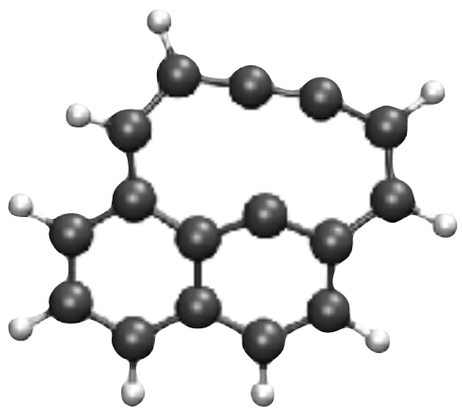
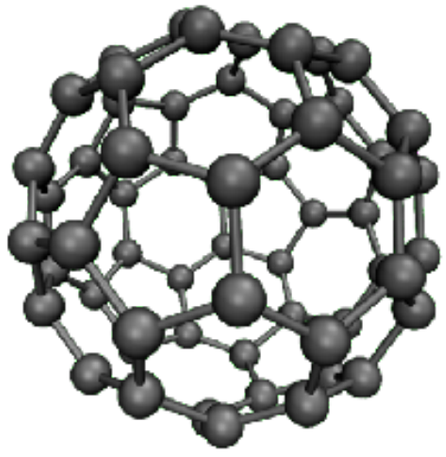
Polycyclic Aromatic Aliphatic Mixed Hydrocarbons

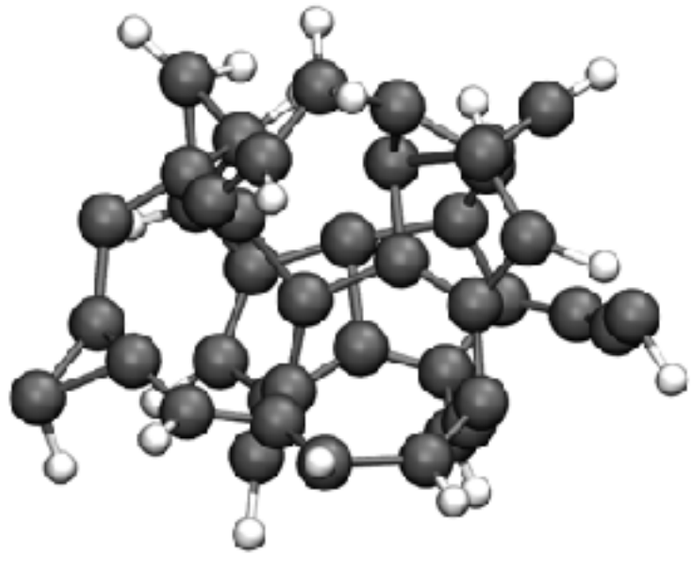












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Objectives

- Explore the diversity of hydrocarbon structures without preconceived model through the use of atomistic simulations
- Compute the spectroscopic response (IR and UV/Visible) of these structures
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We start with carbon clusters C_{24}, C_{42}, and C_{60}

LAMMPS

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⚠ REBO and AIREBO have suffered and still suffer from several issues in LAMMPS

REBO potential

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$$V = \sum_{i<j} \left(V^R(r_{ij}) - b_{ij} V^A(r_{ij}) \right)$$

- b_{ij}: function of the environment of the bond. Includes 3-body and 4-body terms

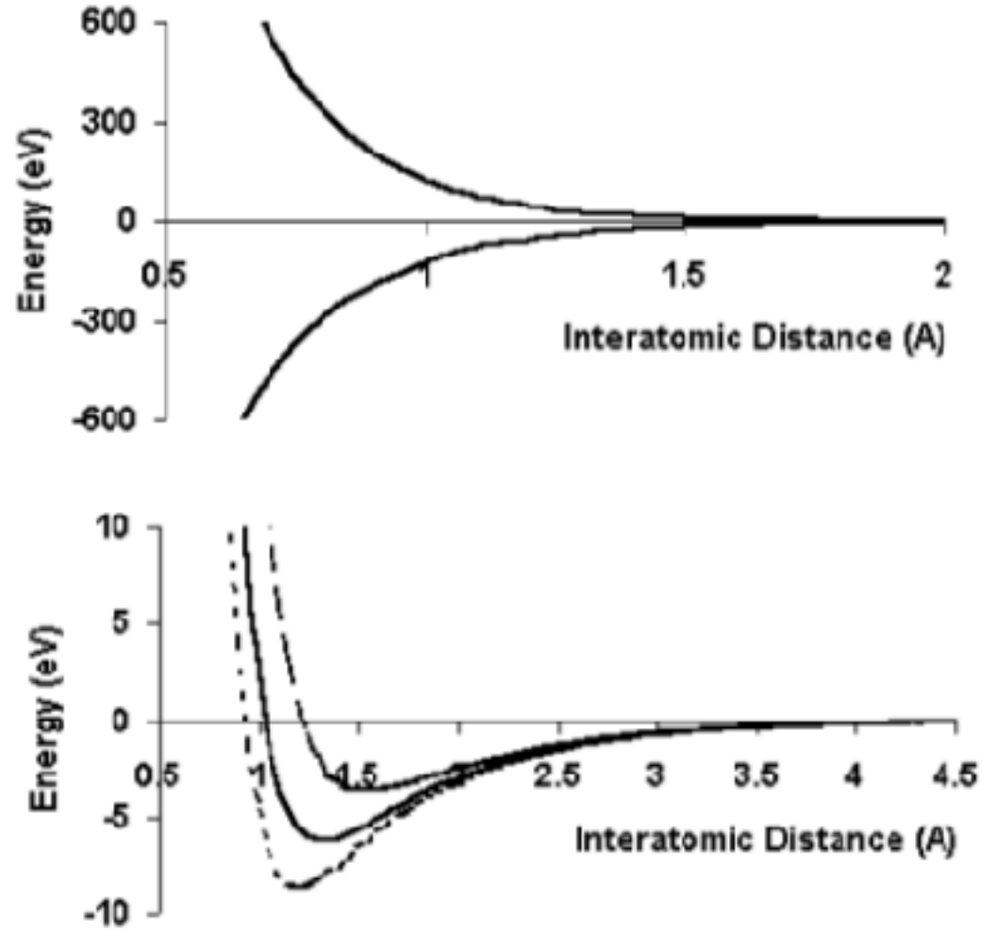

Figure 1. Plots of the pair potentials (5) and (6) obtained using the parameters in table 1. T attractive and repulsive pair terms as a function of interatomic distance. Bottom: pair te triple bonds (dotted curve), double bonds (solid curve), and single bonds (dashed curve) o by multiplying the attractive pair term by the appropriate bond order value and adding i repulsive pair term.

Brenner et al. J. Phys. Cond. Mat., 14, 783 (2002)

AIREBO potential

- AIREBO potential introduced in 2000 by Stuart *Stuart et al., JCP **112** 6472 (2000)*

$$V^{\mathrm{AIREBO}} = V^{\mathrm{REBO}} + V^{\mathrm{LJ}} + V^{\mathrm{Tors}}$$

short-range covalent interactions

non-bonded interactions: Lennard-Jones

torsional potential around single bonds (4-body term)

LAMMPS

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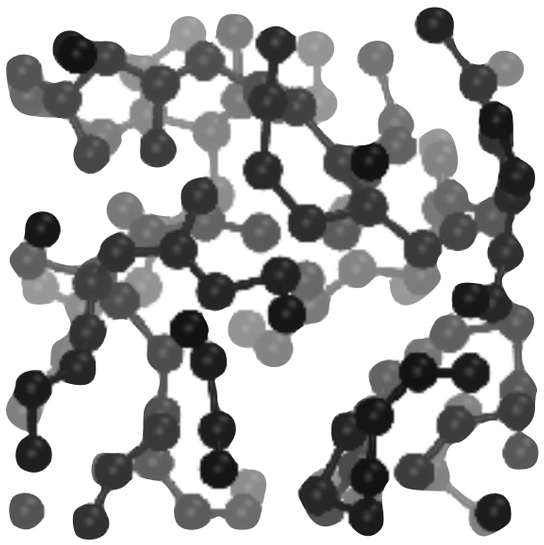
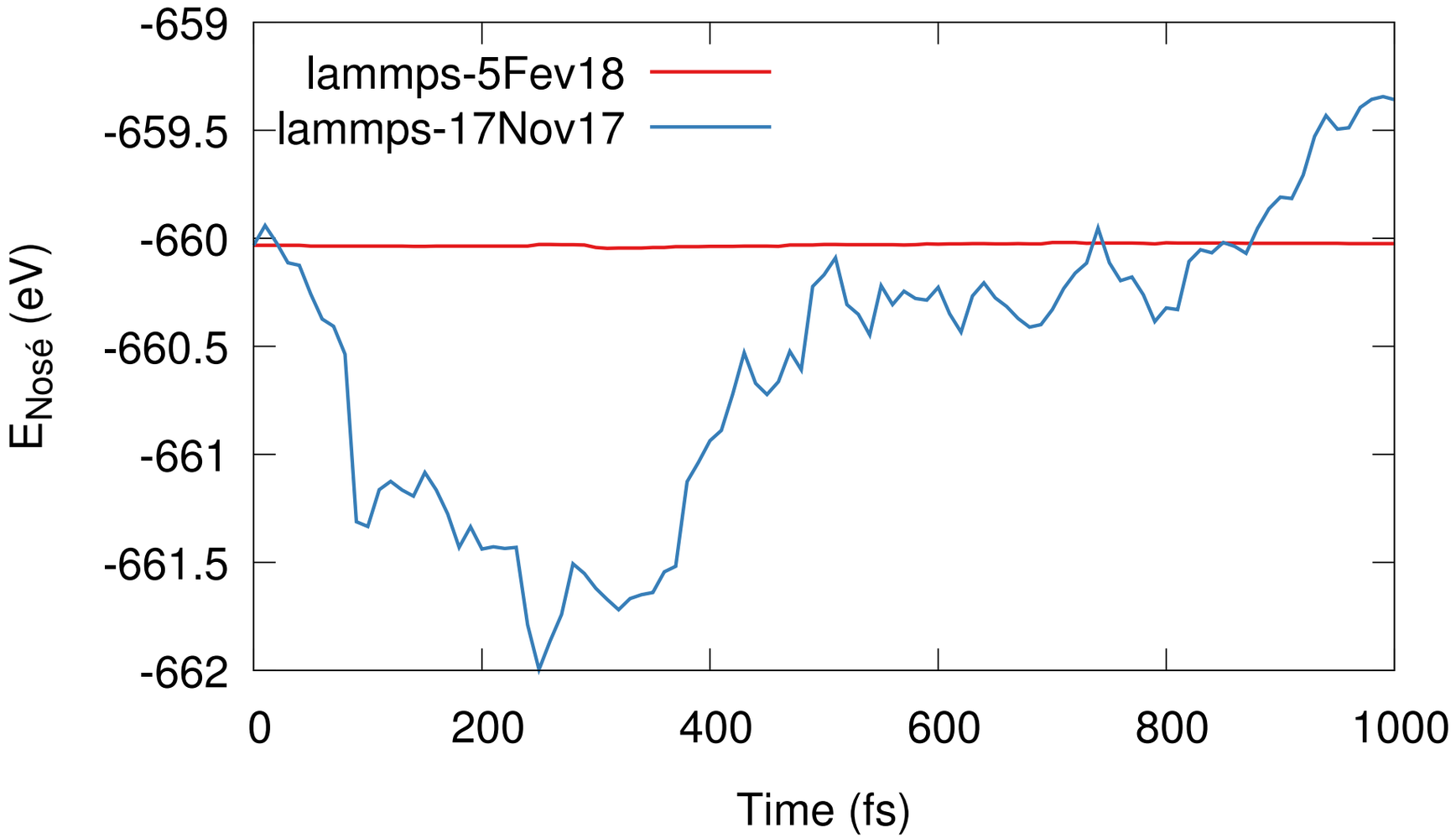
- Trajectories were crashing and energy was not conserved
- Several LAMMPS users/developers contributed to fix several bugs in the force calculation of the (AI)REBO potentials
- With the Aug. 2017 release of LAMMPS these bugs were corrected
  - spline coefficients read from an input file did not correspond to hard-coded parameters
- AIREBO in LAMMPS was implemented from a transcription of a Fortran code which included a bug in the force calculation (LJ part).

Benchmark: liquid carbon

- Box of 128 carbon atoms at 5000 K with PBC (NVT)
  ρ=2 g.cm^{-3}, Δt=0.01 fs





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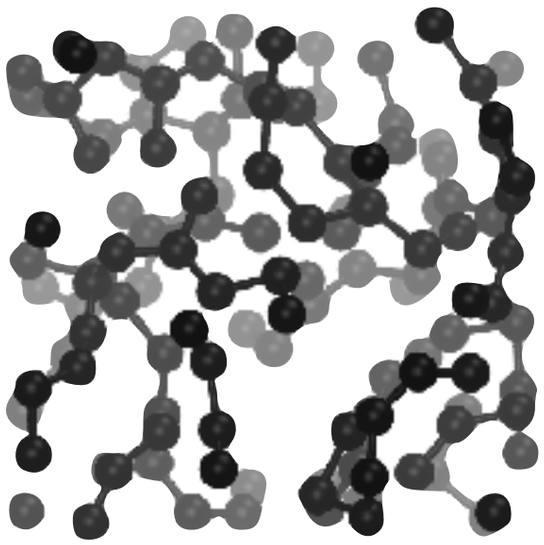

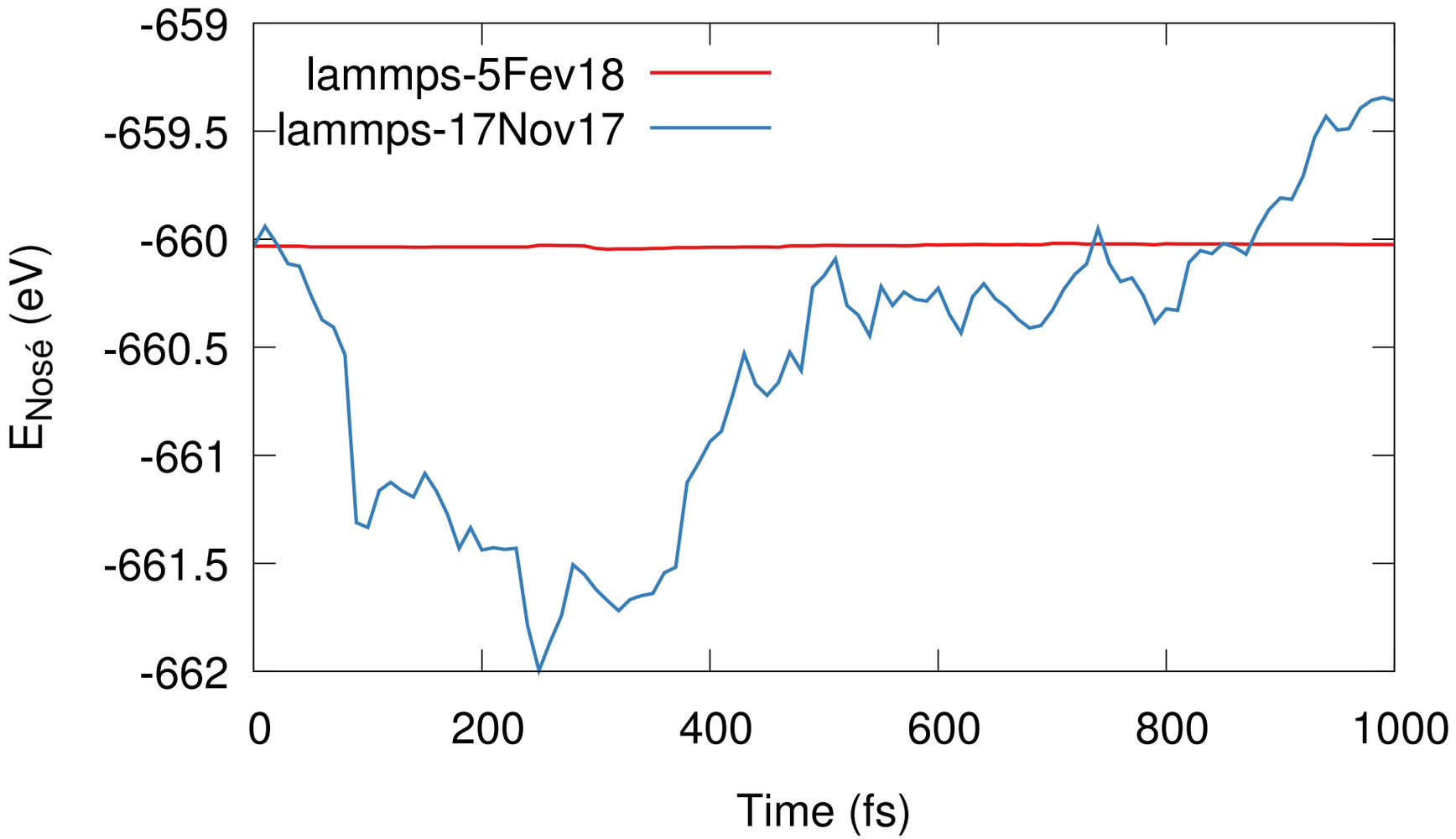

Can we now safely use AIREBO with LAMMPS ?

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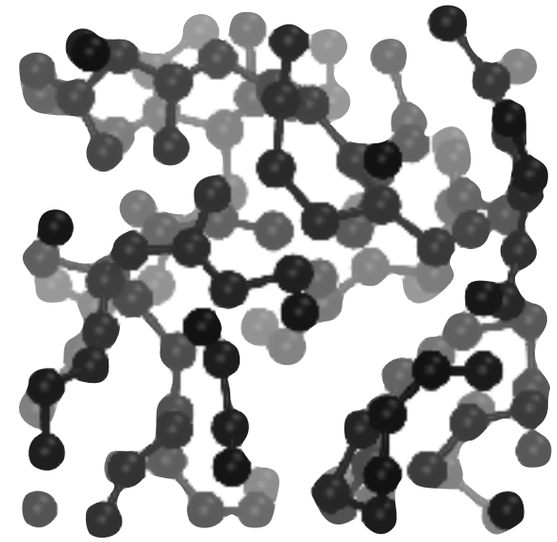

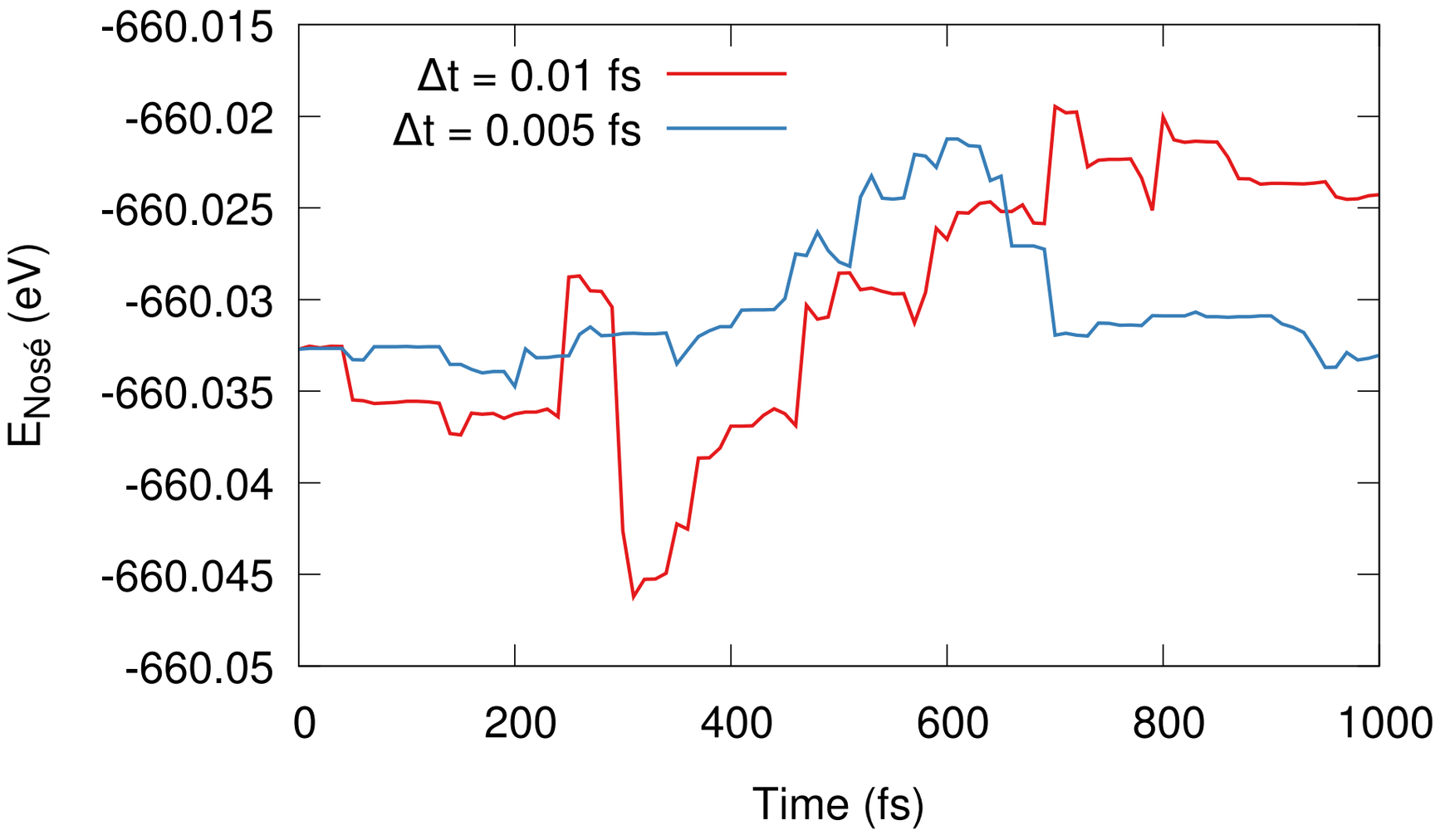

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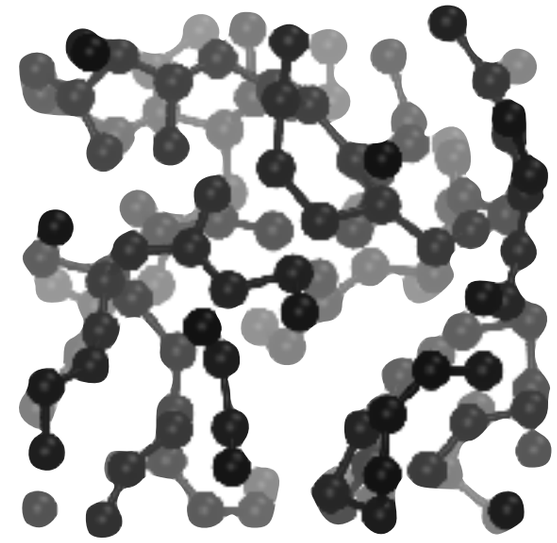

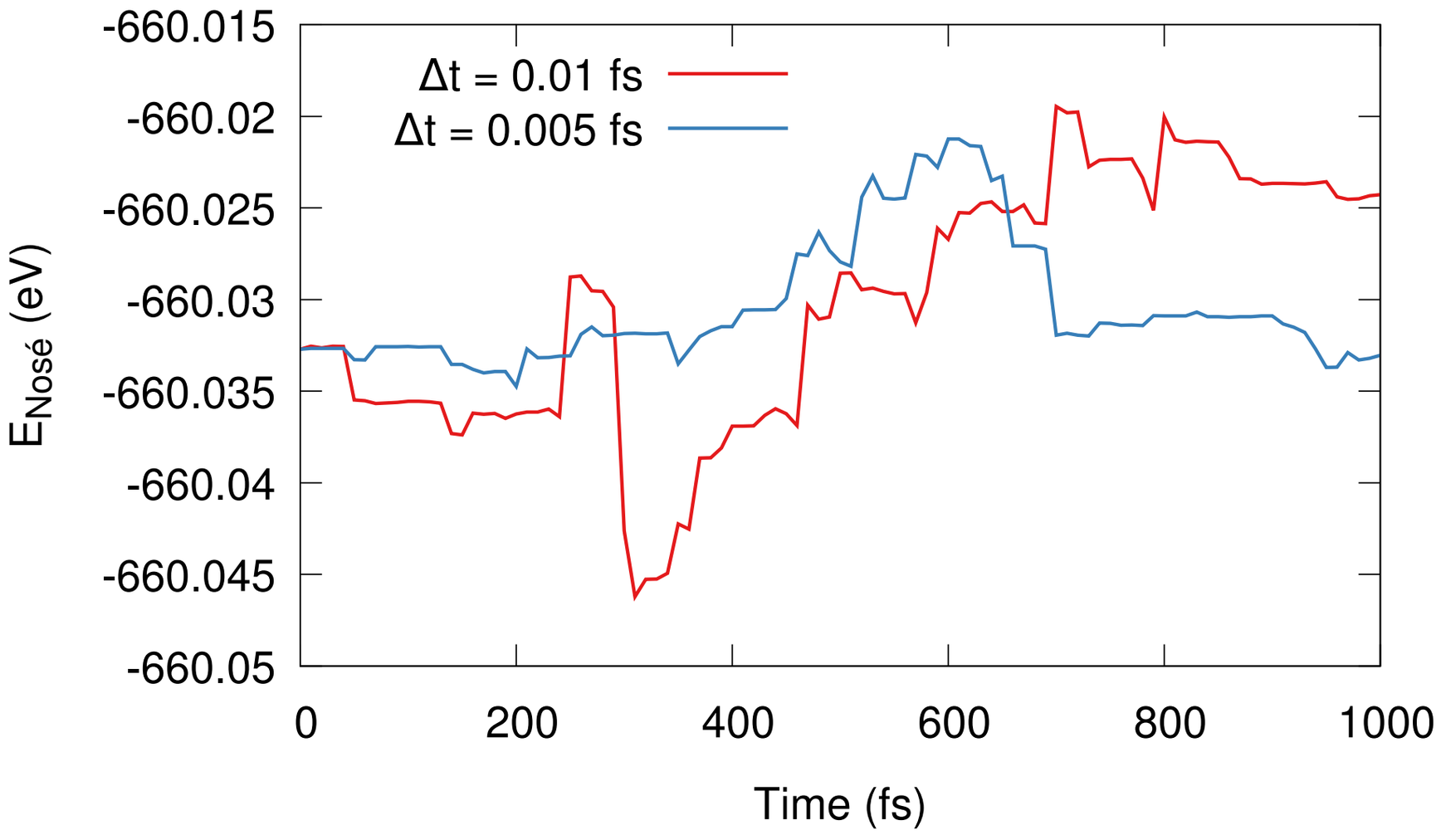

Energy jumps remain even at very small timesteps

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$w_{ij}(r_{ij})$ REBO cutoff for short range interactions

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- Smooth version of the connectivity switch

$$C_{ij} = (1 - w_{ij}) \prod_{k \neq i,j} (1 - w_{ik}w_{kj}) \prod_{k,l \neq i,j} (1 - w_{ik}w_{kl}w_{lj})$$

⚠ this function has not been properly tested

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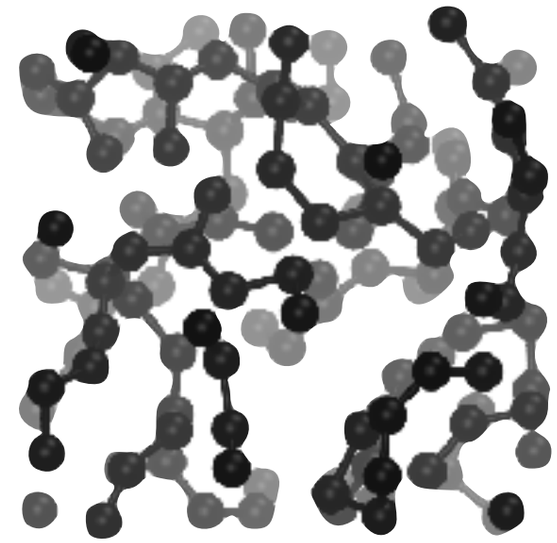

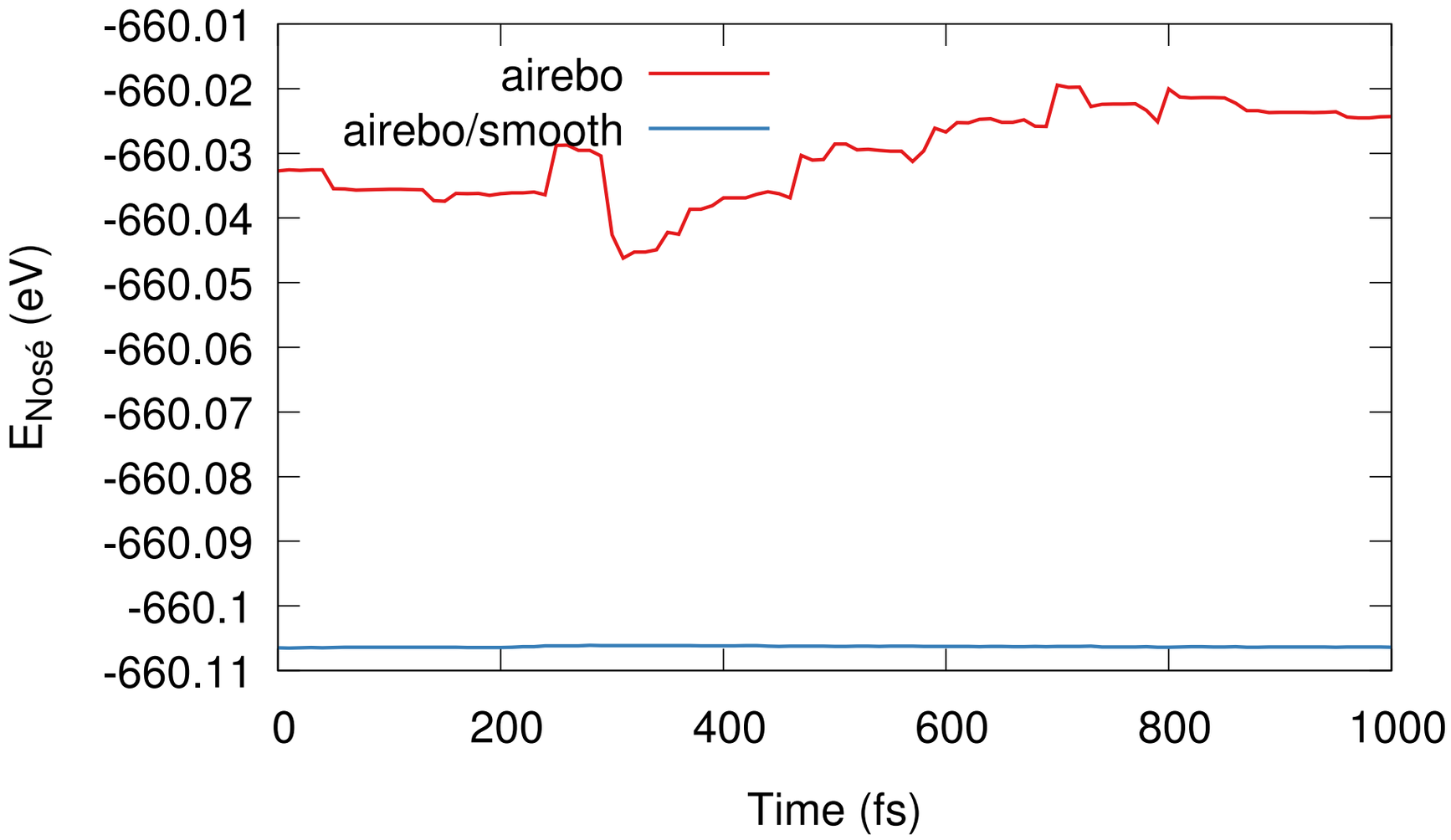

Energy conservation is finally recovered !

LAMMPS

AIREBO

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Ethylene	-24.4077	-24.5284	-24.4077
Cyclopropene	-28.2589	-28.3610	-28.2589
Allene	-30.2392	-30.3511	-30.2392
Propene	-37.3047	-37.5116	-37.3047
Cyclobutene	-42.1801	-42.3536	-42.1797
1,3-Butadiene	-43.0035	-43.3977	-43.0035
1-Butene	-50.0487	-50.2557	-50.0486
2-Butene	-50.2017	-50.4951	-50.2016
1,4-Pentadiene	-56.5078	-56.9220	-56.5079
Cyclopentene	-57.1119	-57.3895	-57.1121
2-Methyl-1-butene	-62.9658	-63.0254	-62.9658
2-Methyl-2-butene	-63.1109	-63.2642	-63.1188
Benzene	-59.3096	-60.2313	-59.3096
Naphthalene	-93.8784	-95.0955	-93.8785

REBO: potential given in distributed version of LAMMPS (02/2018)

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1-Butene	-50.0487	-50.2557	-50.0486
2-Butene	-50.2017	-50.4951	-50.2016
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average error for REBO: 335 meV

average error for REBO': 2 meV

Potential energy surface exploration of carbon clusters

LAMMPS

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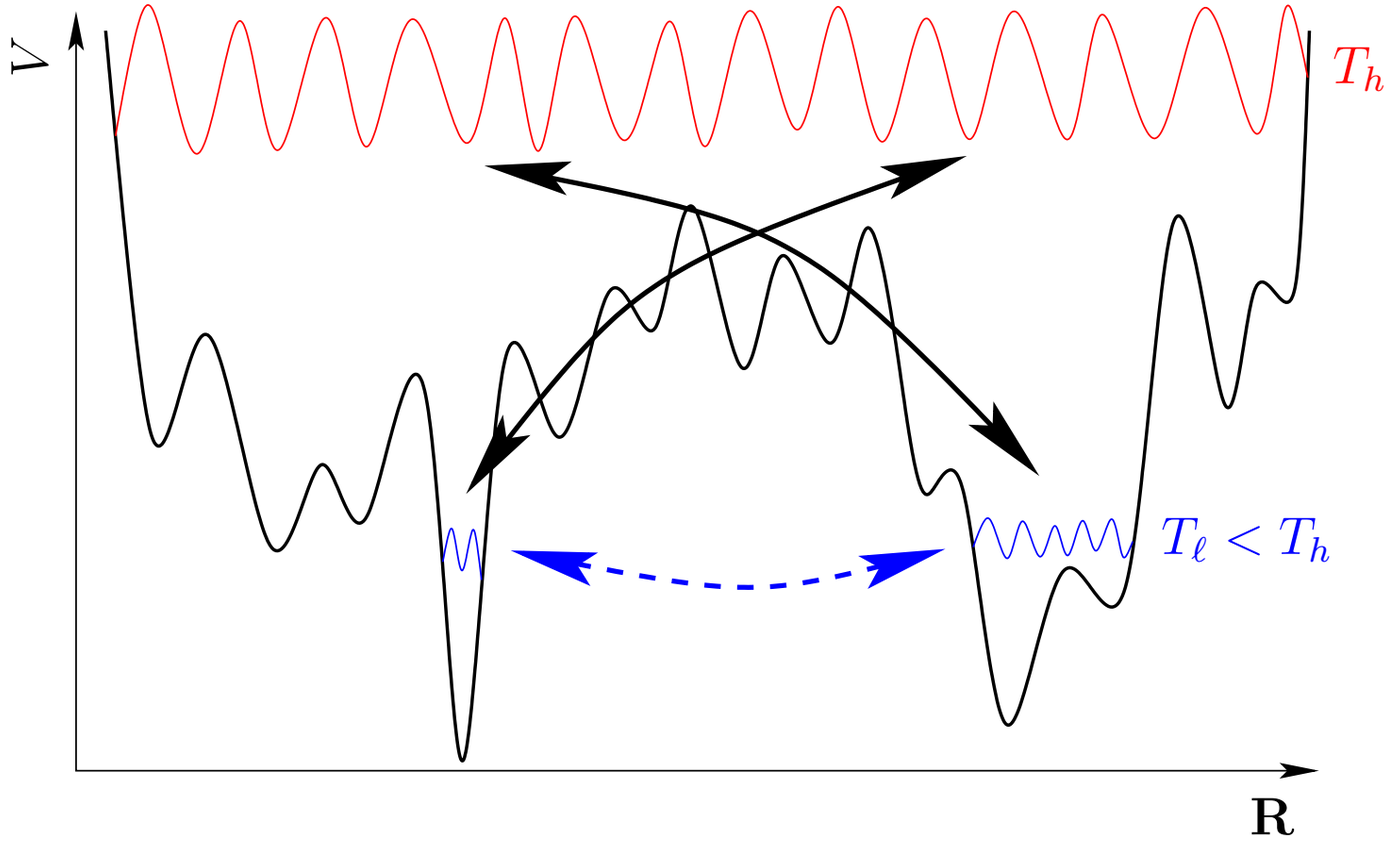
Use of Replica Exchange Molecular Dynamics (REMD) simulations



LAMMPS

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Cluster	T_{min} (K)	T_{max} (K)	N_{temp}	R_{min} (Å)	R_{max} (Å)
C_{24}	1500	6500	12	4.1	16.6
C_{42}	2500	6500	14	4.9	20.0
C_{60}	2500	6500	16	5.5	22.5

LAMMPS

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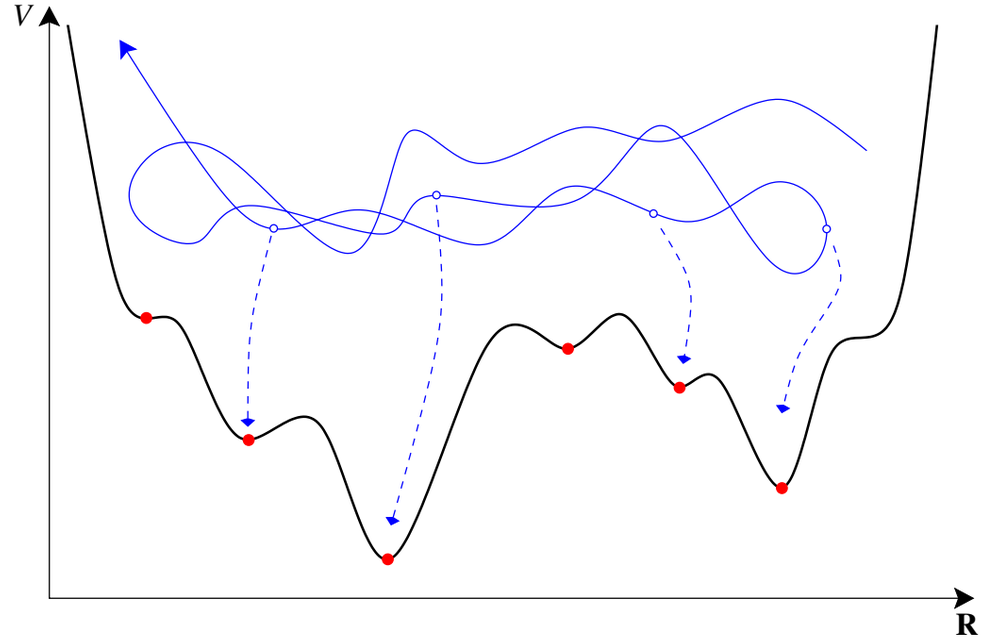
C_{42}	2500	6500	14	4.9	20.0
C_{60}	2500	6500	16	5.5	22.5

- Quenching of the structures to extract local minima
- Elimination of redundant structures and dissociated structures



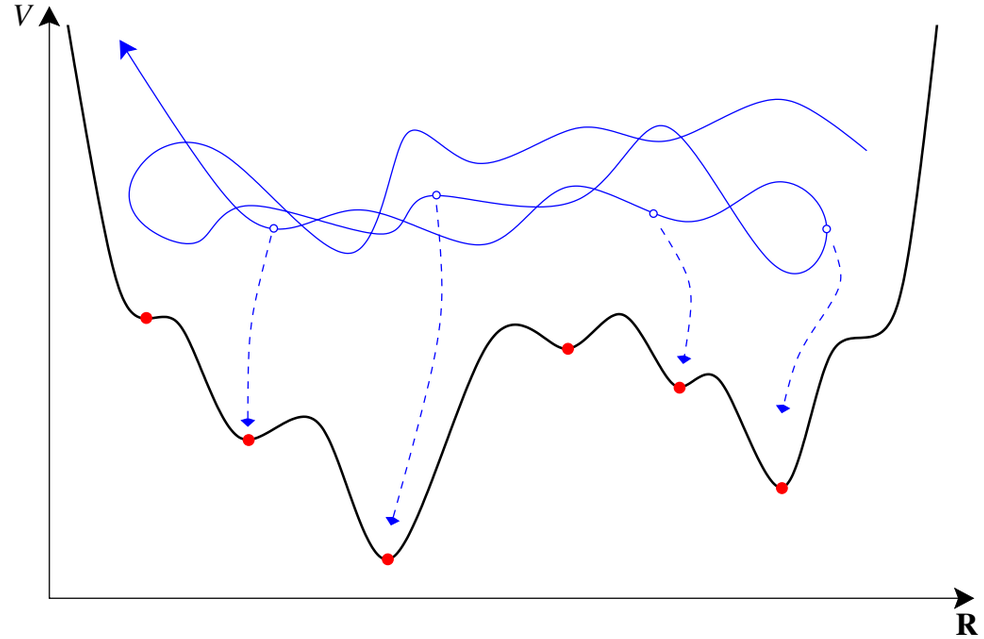
LAMMPS

Simulation protocol

- REMD simulation over a wide range of temperature T~2000 K — 6500 K using REBO
- Use of spherical boundary conditions with various densities ρ=0.025 g/cm³ — 1.7 g/cm³

Cluster	T_{min} (K)	T_{max} (K)	N_{temp}	R_{min} (Å)	R_{max} (Å)
C_{24}	1500	6500	12	4.1	16.6
C_{42}	2500	6500	14	4.9	20.0
C_{60}	2500	6500	16	5.5	22.5

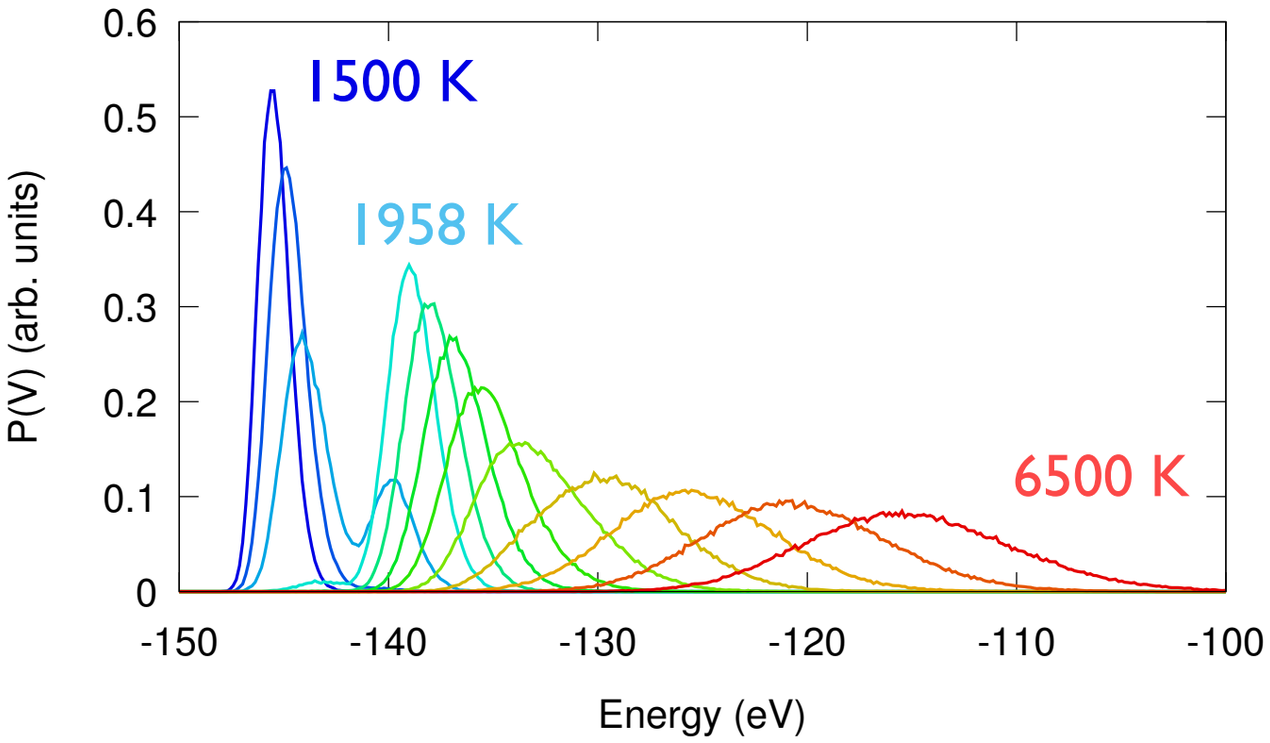
- Quenching of the structures to extract local minima
- Elimination of redundant structures and dissociated structures



Cluster	before selection	dissociated	redundant	final
C_{24}	1,500,060	149,933	1,251,764	98,363
C_{42}	1,400,056	282,204	631,380	486,472
C_{60}	1,600,064	320,332	623,294	656,438

LAMMPS

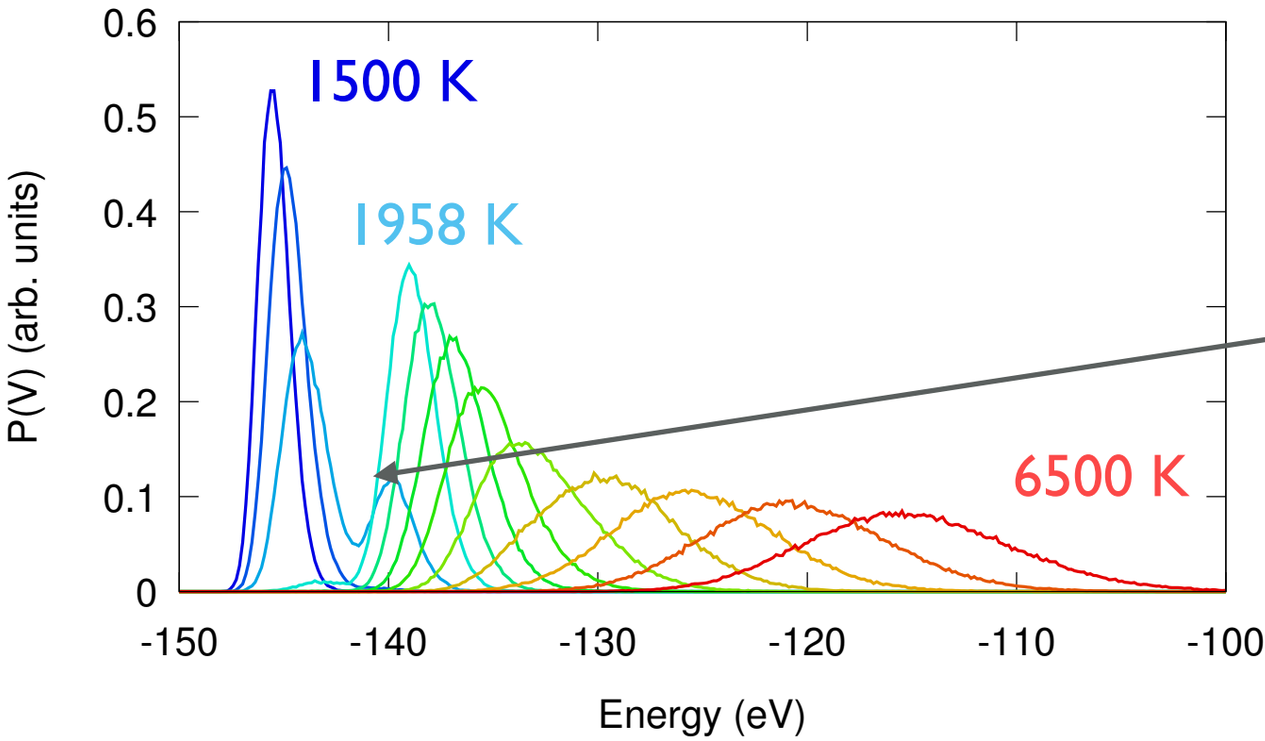
C_{24}: example of REMD simulation



ρ=0.15 g/cm³, R=9.1 Å

LAMMPS

C_{24}: example of REMD simulation

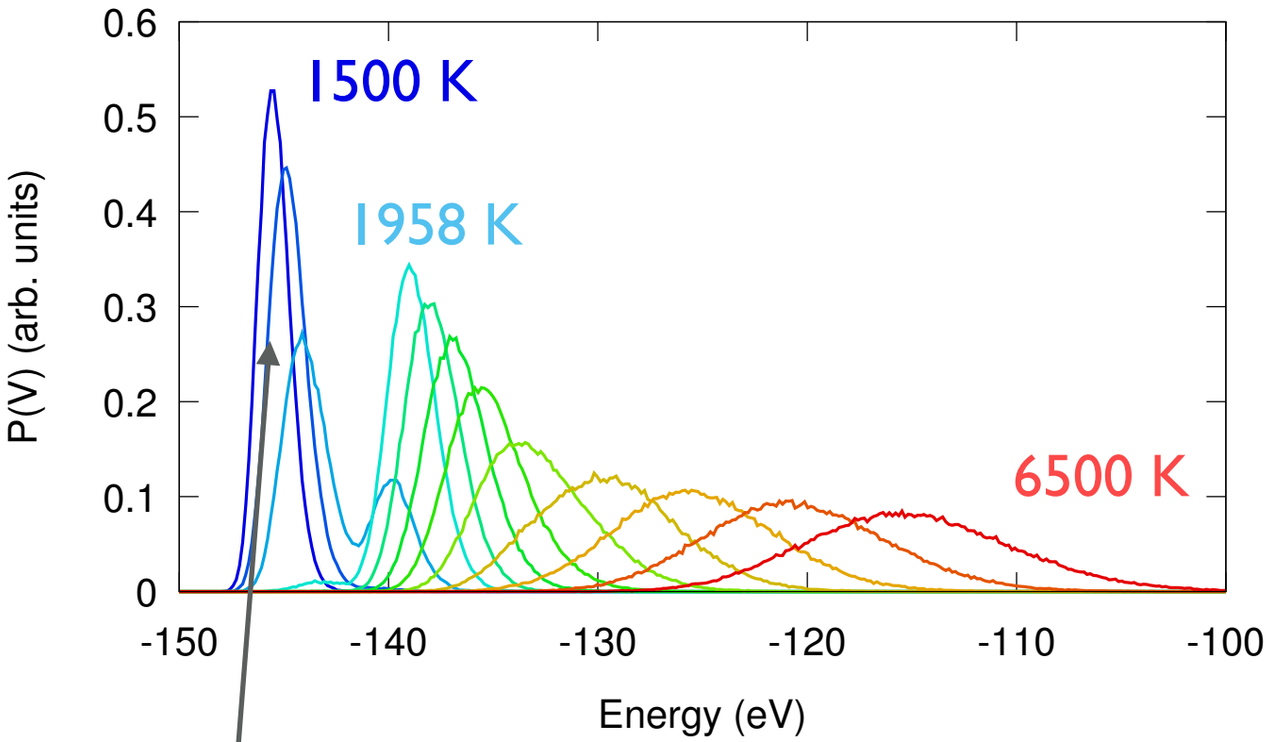


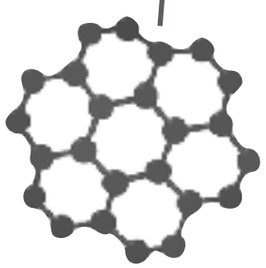
ρ=0.15 g/cm^3, R=9.1 Å

phase transition

LAMMPS

C_{24}: example of REMD simulation



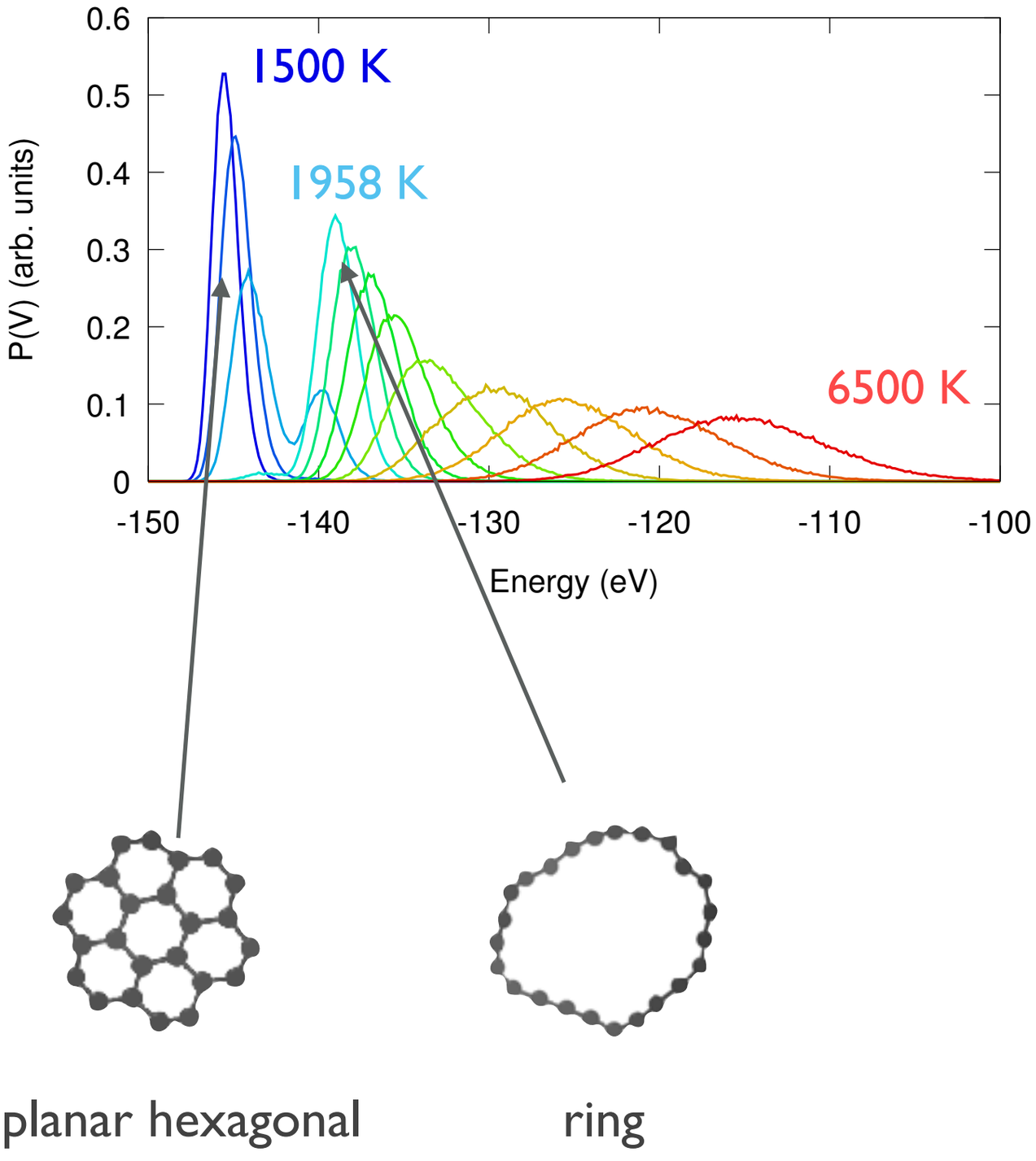


planar hexagonal

ρ=0.15 g/cm^3, R=9.1 Å

LAMMPS

C_{24}: example of REMD simulation



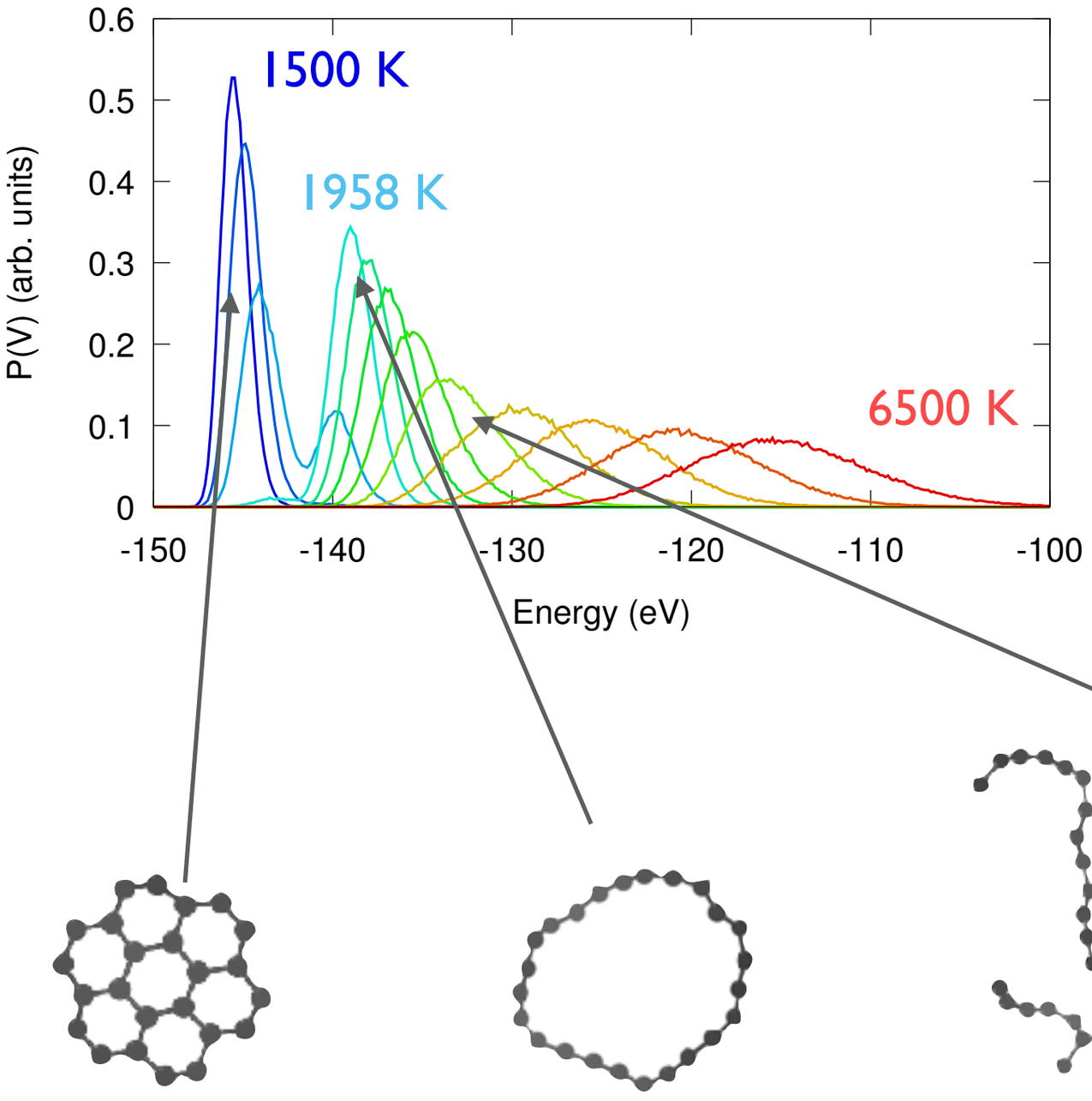
planar hexagonal

ring

ρ=0.15 g/cm^3, R=9.1 Å

LAMMPS

C_{24}: example of REMD simulation



ρ=0.15 g/cm^3, R=9.1 Å

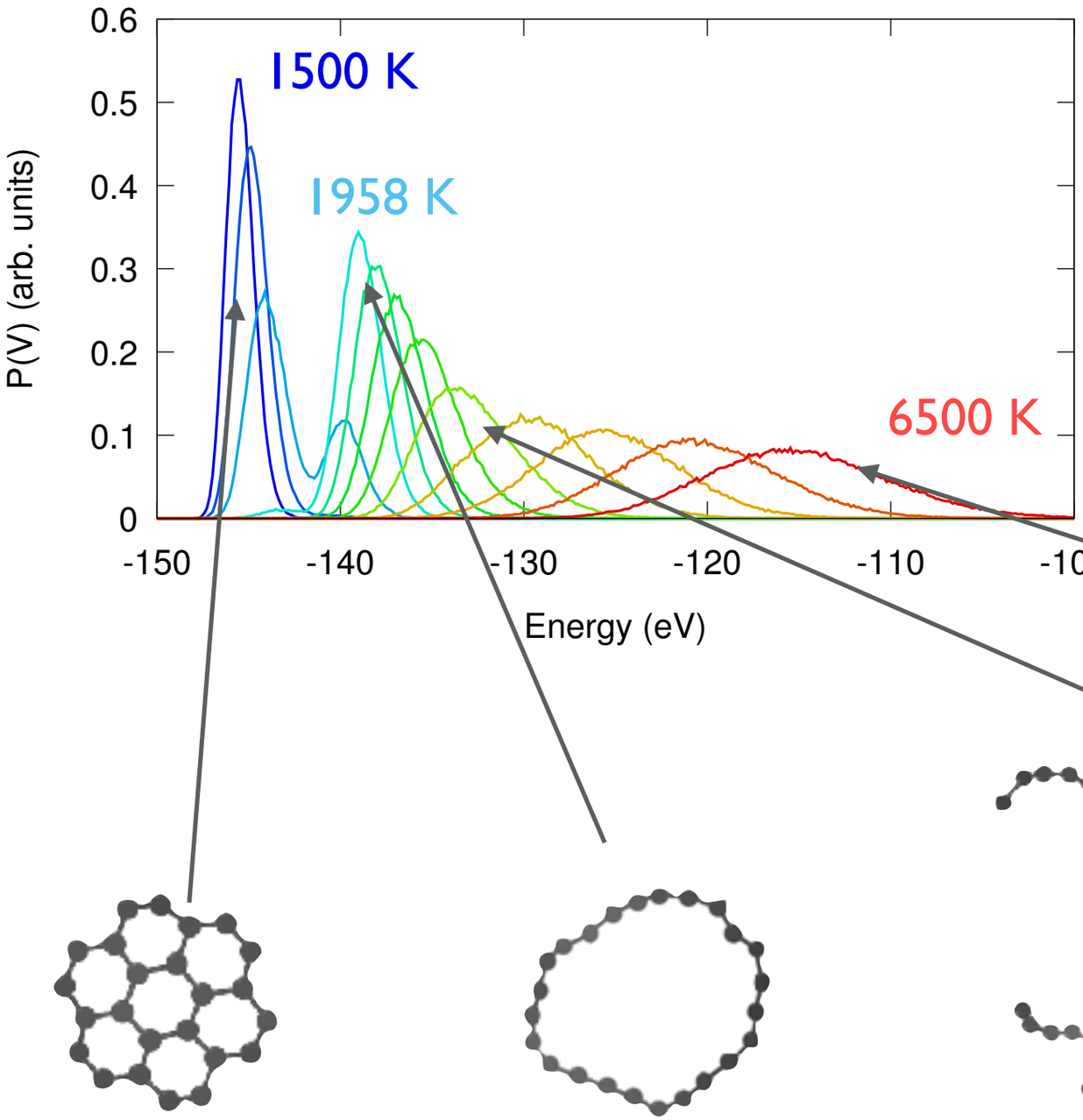
planar hexagonal

ring

open + bretzel

LAMMPS

C_{24}: example of REMD simulation

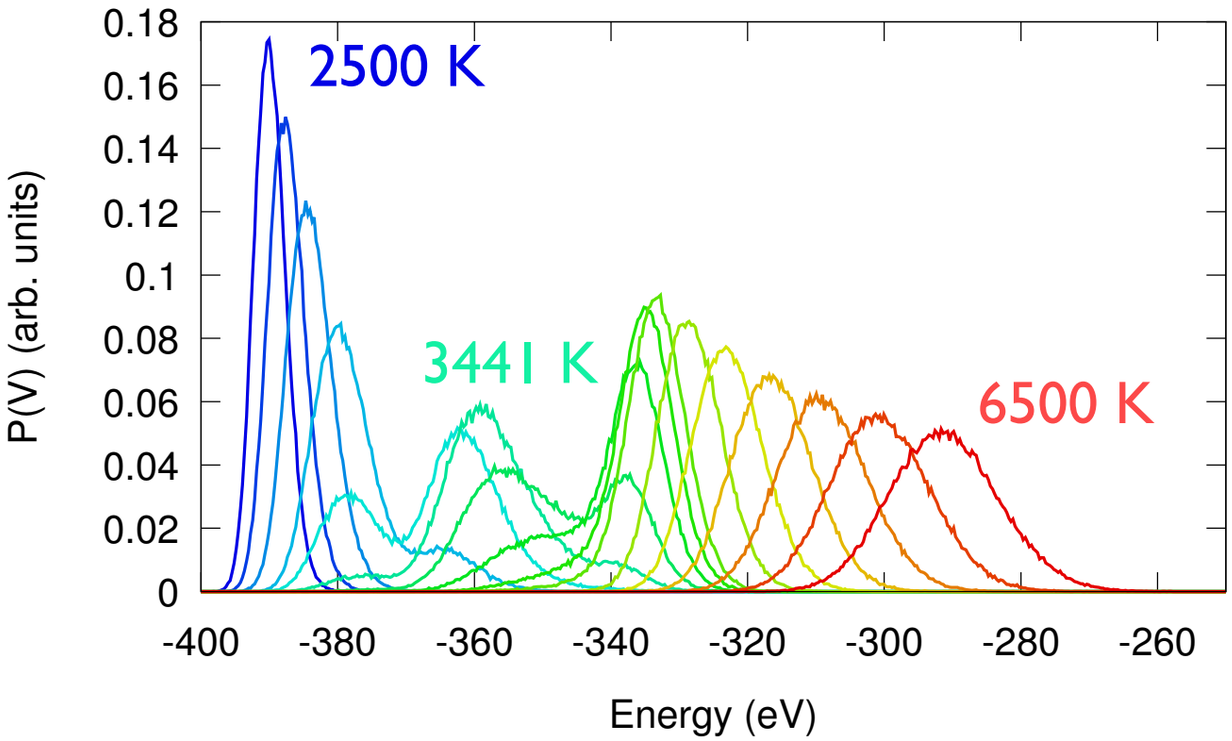


ρ=0.15 g/cm³, R=9.1 Å

planar hexagonal | ring | open + bretzel | dissociated

LAMMPS

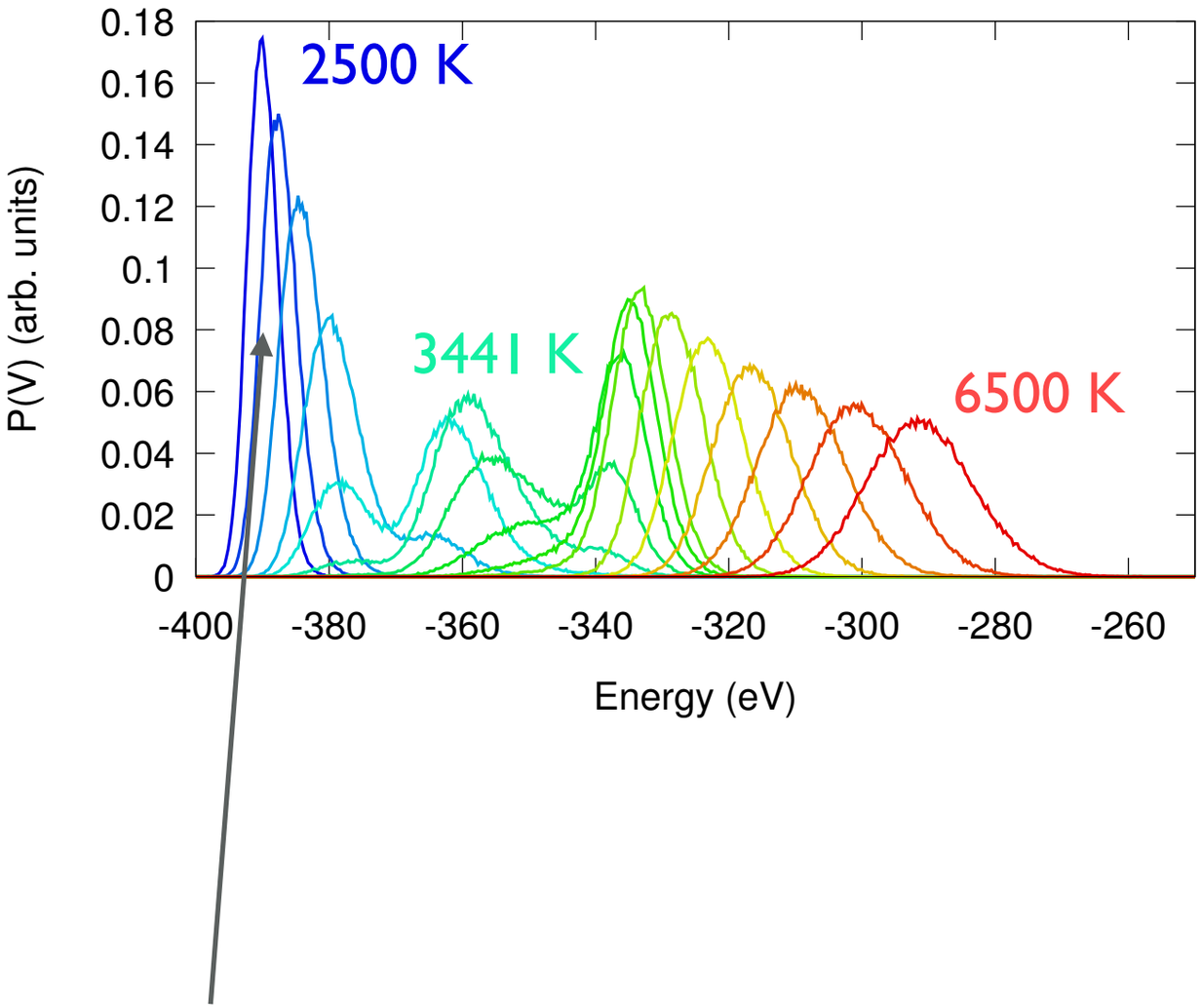
C_{60}: example of REMD simulation

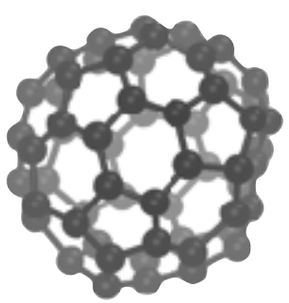


ρ=0.15 g/cm³, R=12.4 Å

LAMMPS

C_{60}: example of REMD simulation



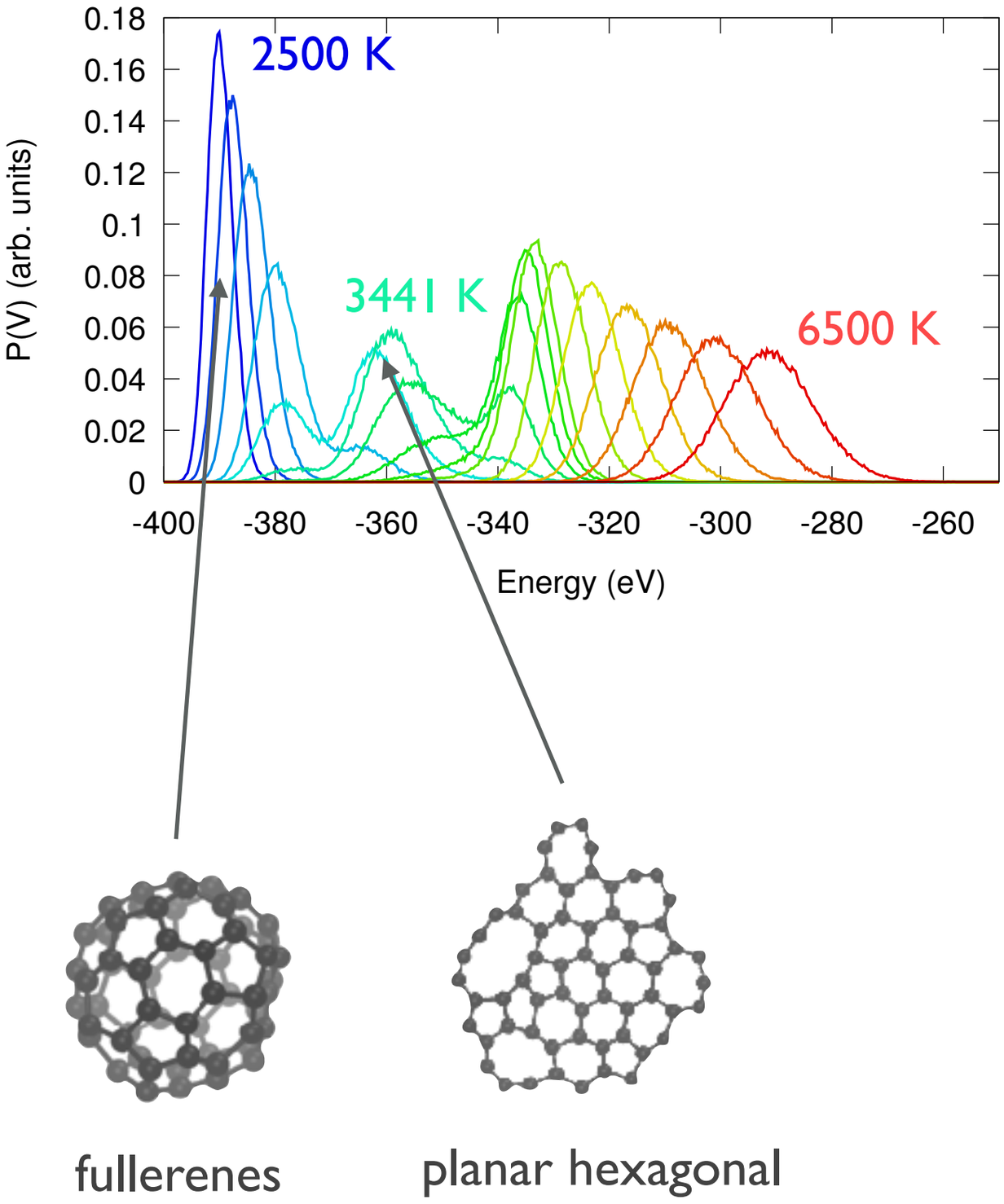


fullerenes

ρ=0.15 g/cm³, R=12.4 Å

LAMMPS

C_{60}: example of REMD simulation



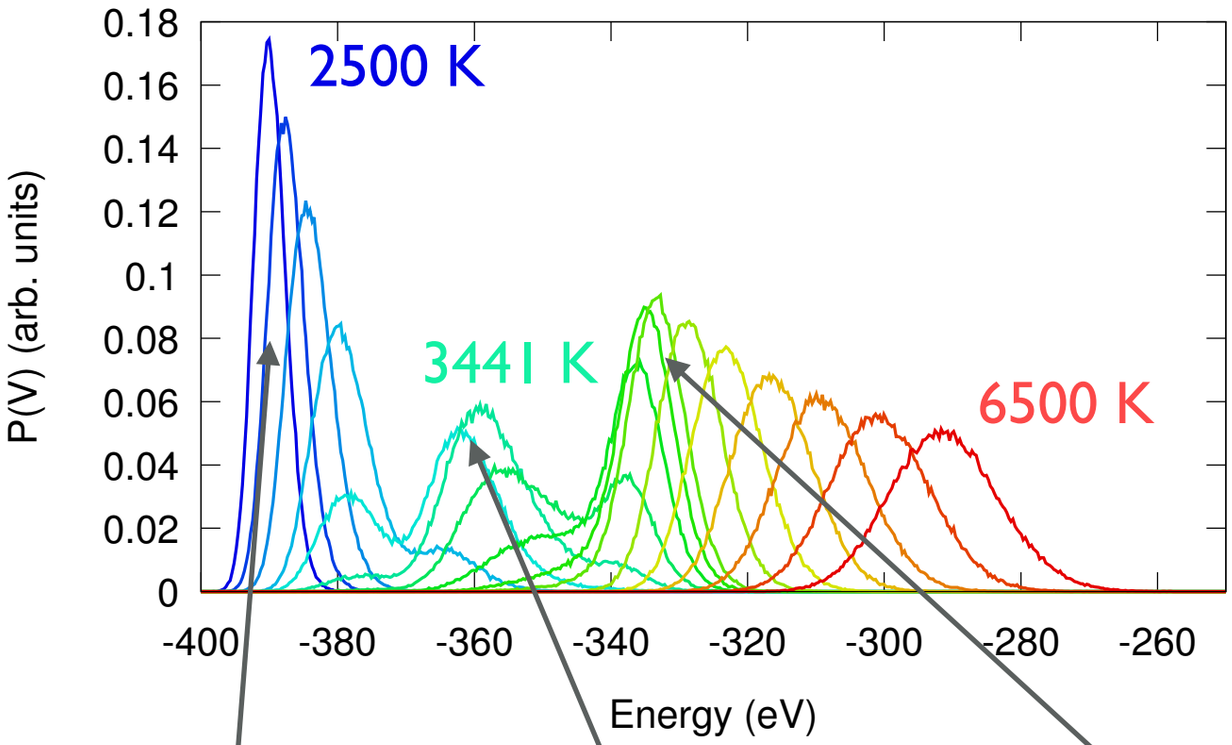
fullerenes

planar hexagonal

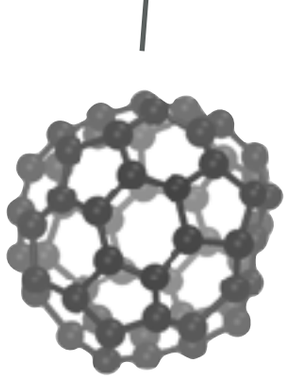
ρ=0.15 g/cm³, R=12.4 Å

LAMMPS

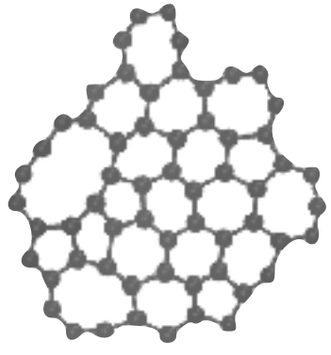
C_{60}: example of REMD simulation



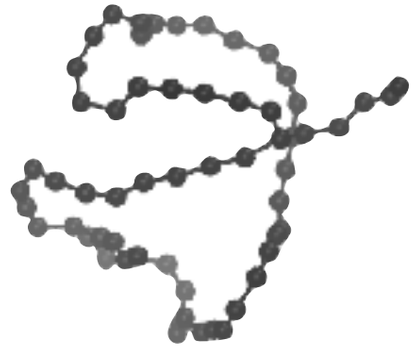
ρ=0.15 g/cm³, R=12.4 Å



fullerenes



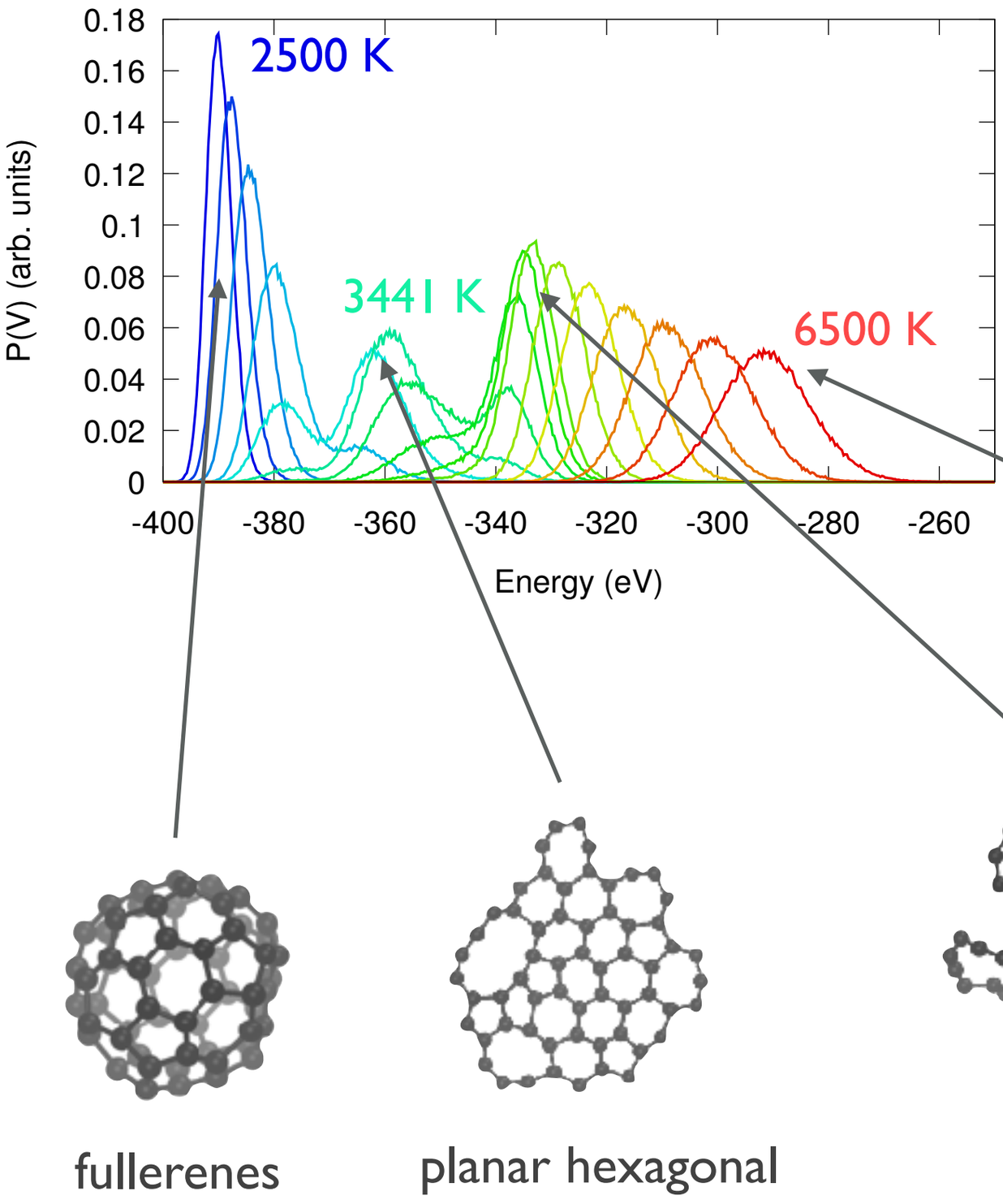
planar hexagonal



bretzel

LAMMPS

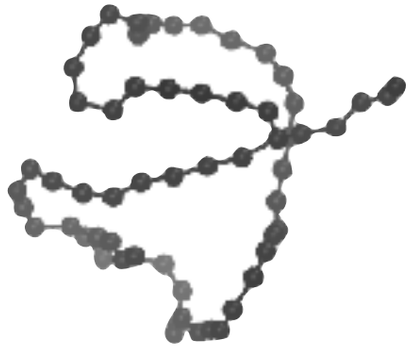
C_{60}: example of REMD simulation



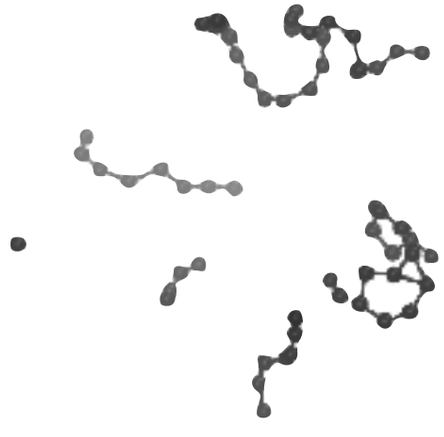
ρ=0.15 g/cm³, R=12.4 Å

fullerenes

planar hexagonal



bretzel



dissociated

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Structural analysis

- Gyration tensor $Q^{\alpha\beta} = \frac{1}{N}\sum_i \delta r_i^\alpha \delta r_i^\beta \qquad \delta\mathbf{r}_i = \mathbf{r}_i - \mathbf{r}_g$

$R_g^2 = \frac{1}{N}\sum_i \delta\mathbf{r}_i^2 = \mathrm{Tr}\mathbf{Q}$ squared radius of gyration: spatial extension of the structure

$\mathbf{D} = \mathbf{Q} - \mathrm{Tr}\mathbf{Q}\ \mathbf{I}$

$A_3 = \frac{3}{2}\frac{\mathrm{Tr}\left(\mathbf{D}^2\right)}{\left(\mathrm{Tr}\mathbf{Q}\right)^2}$ asphericity: A_3=0 for a sphere, A_3=1 for a linear chain

$S = 27\frac{\mathrm{Det}\left(\mathbf{D}\right)}{\left(\mathrm{Tr}\mathbf{Q}\right)^3}$ prolateness: S=-0.25 for a plane, S=2 for a linear chain

- Hybridization state: purely geometrical definition from the number of neighbors and the angles

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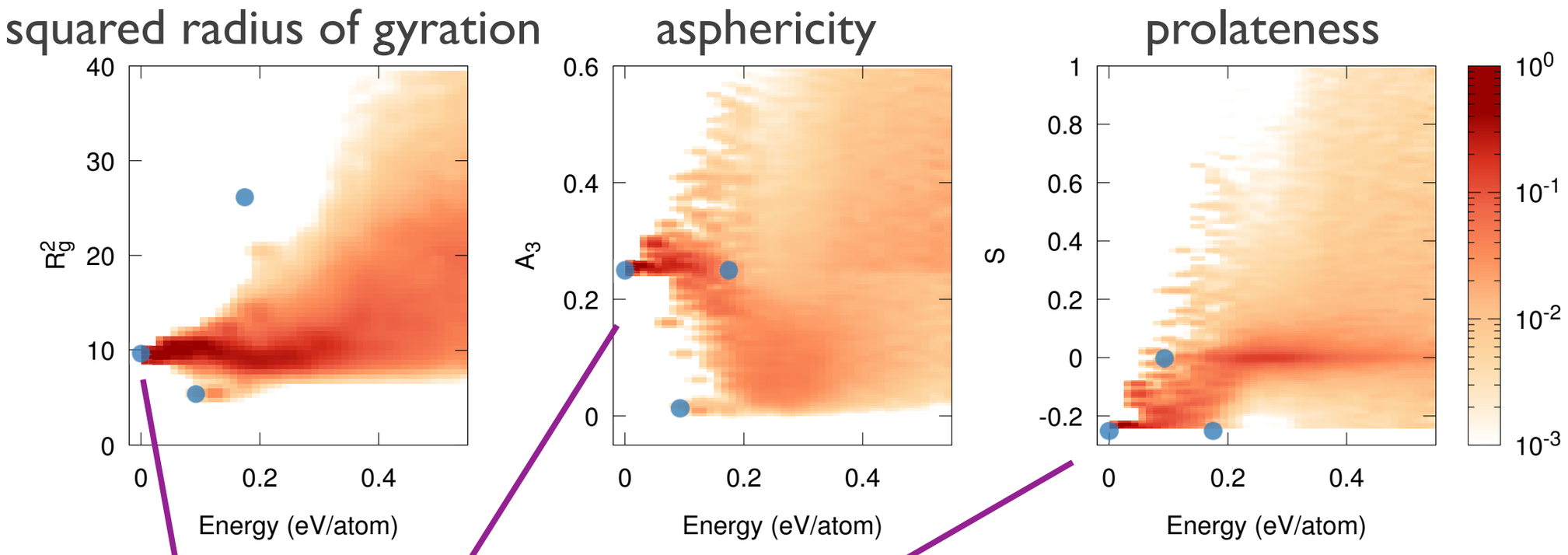
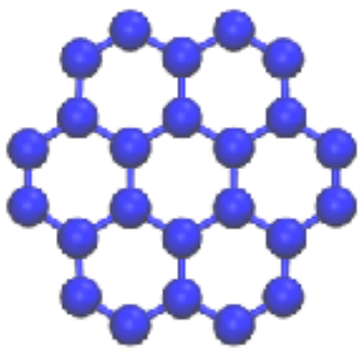
Analysis of the quenched structures: C_{24}





dehydrocoronene

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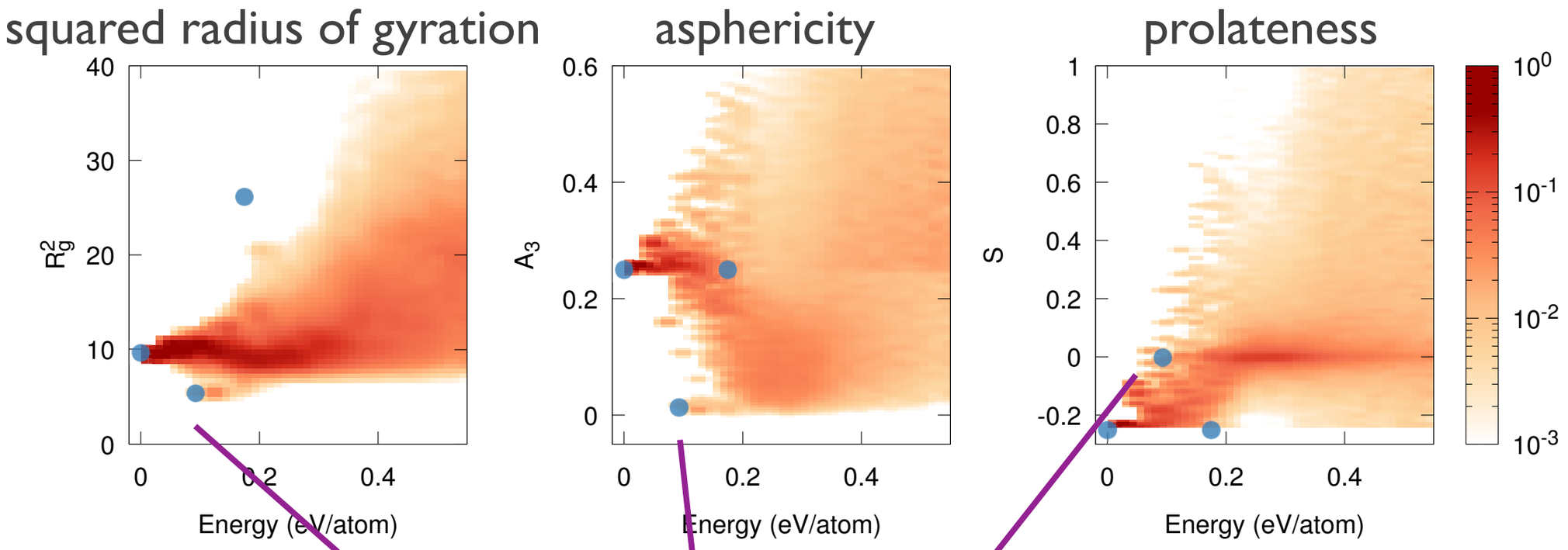
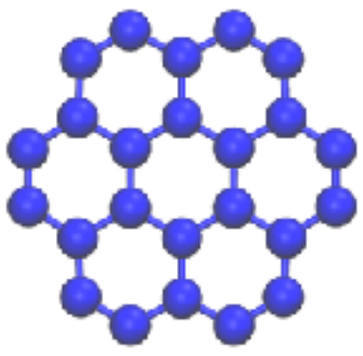
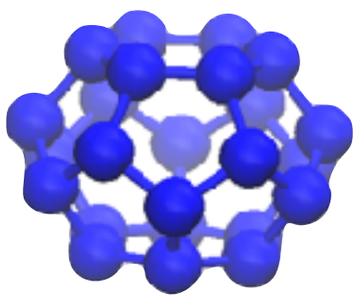
Analysis of the quenched structure: C_{24}





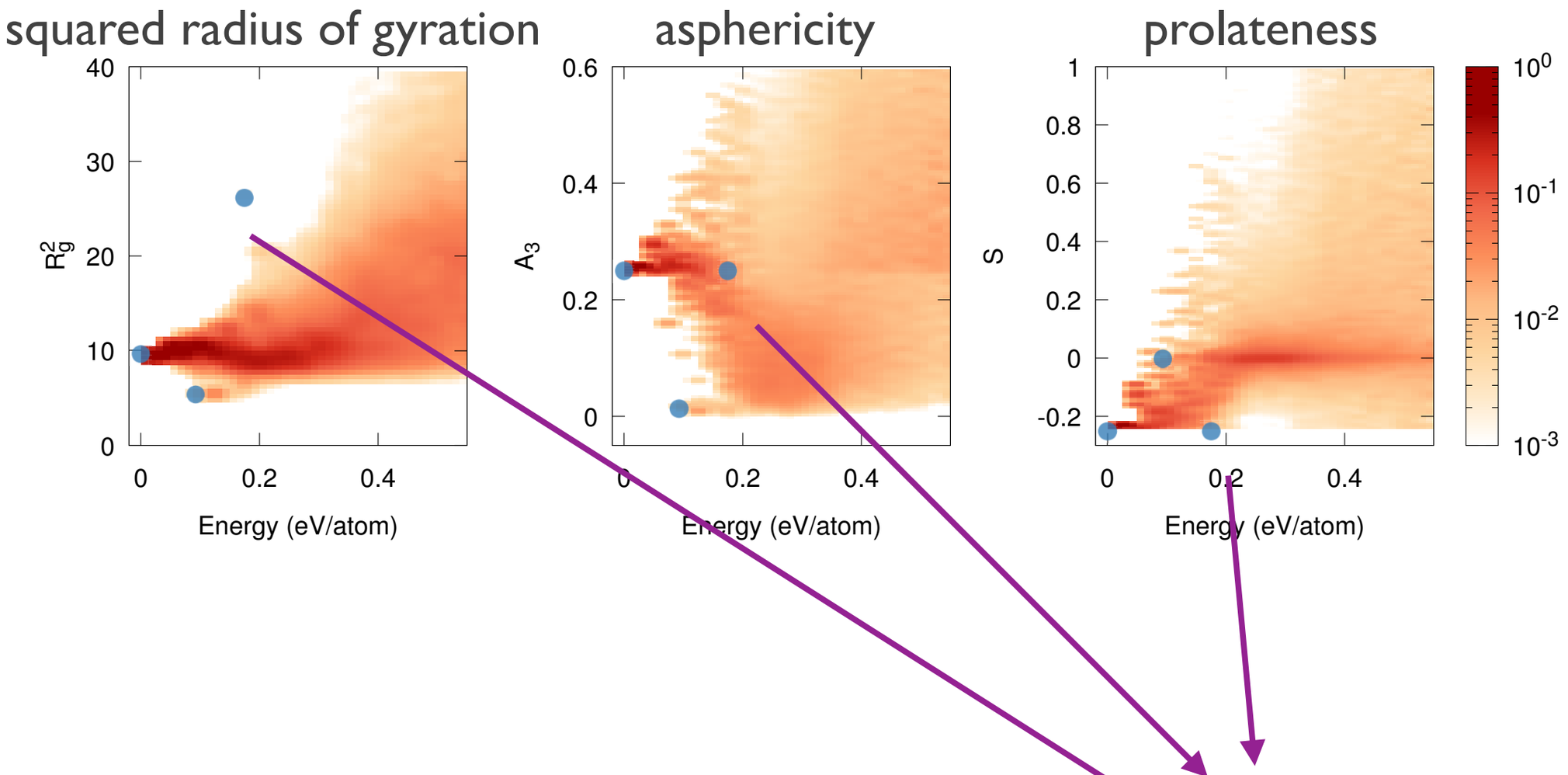
dehydrocoronene

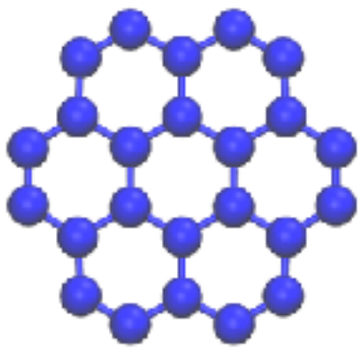


fullerene

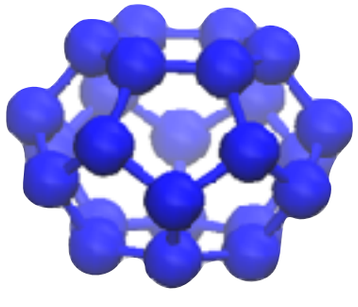
LAMMPS

Analysis of the quenched structure: C_{24}

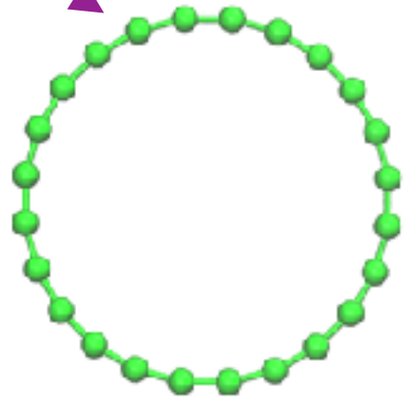




dehydrocoronene



fullerene

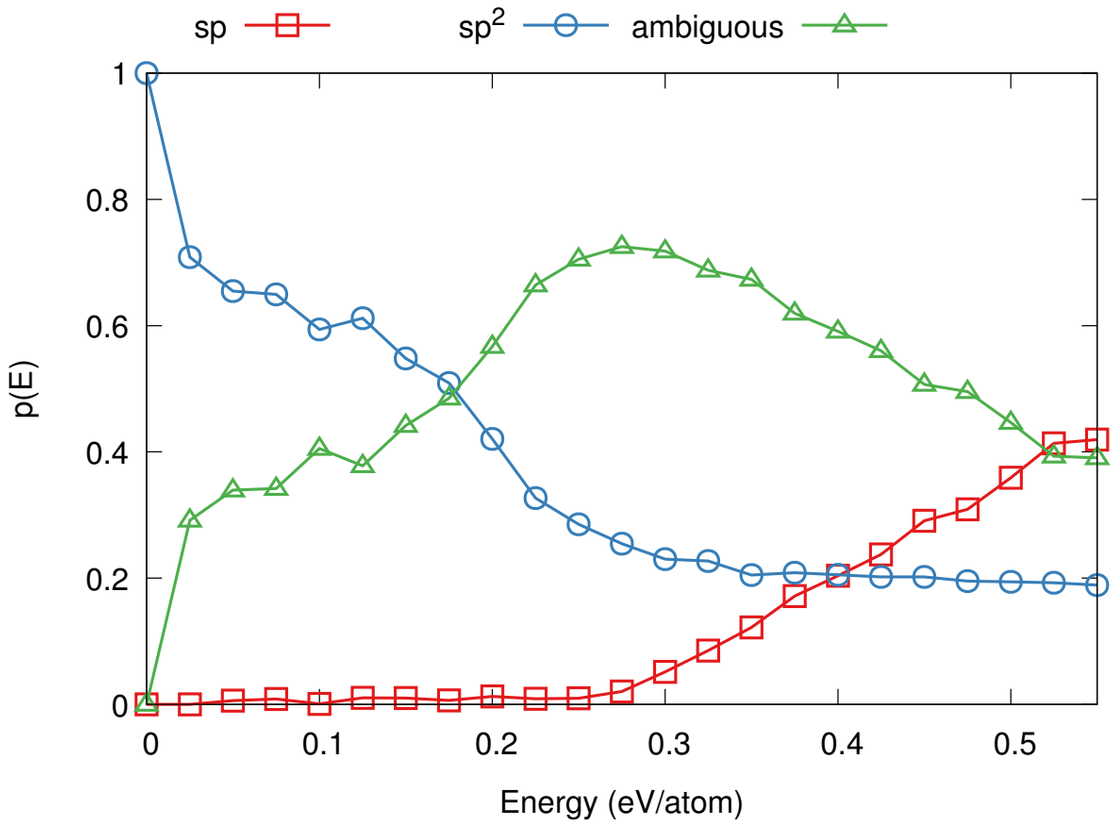


ring

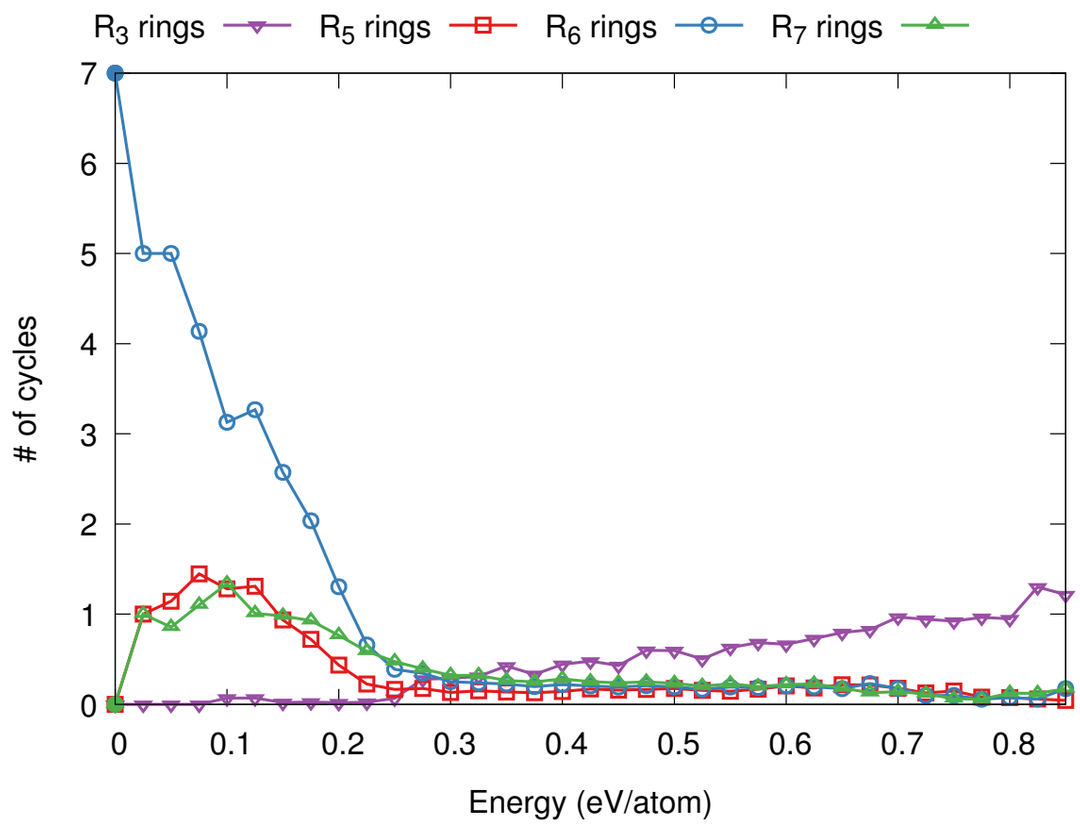
LAMMPS

Analysis of the quenched structure: C_{24}

hybridization state



of cycles



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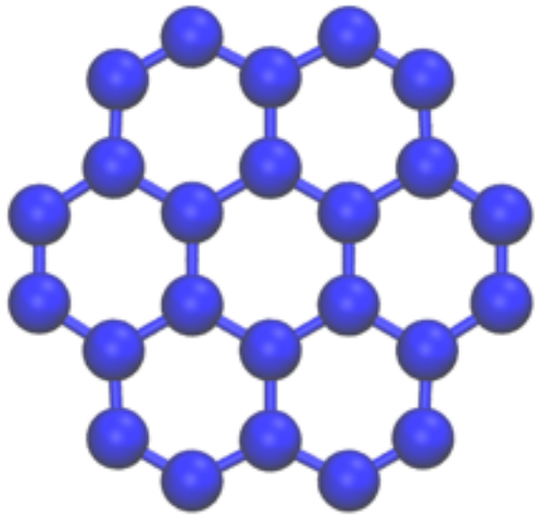
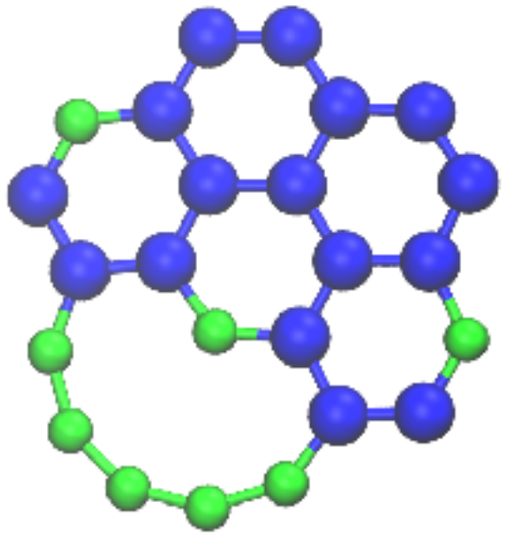
Analysis of the quenched structures: C_{24}

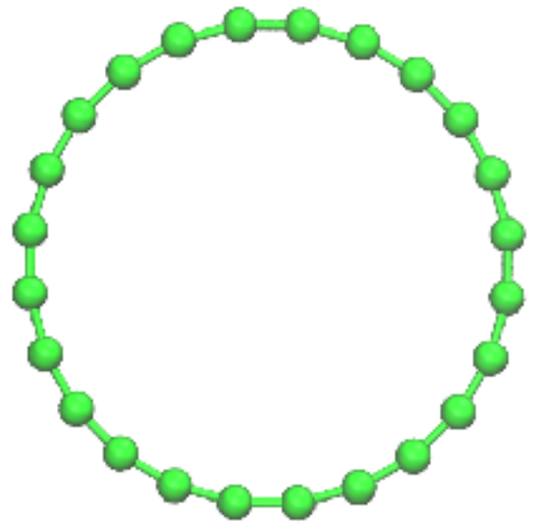
E = 0



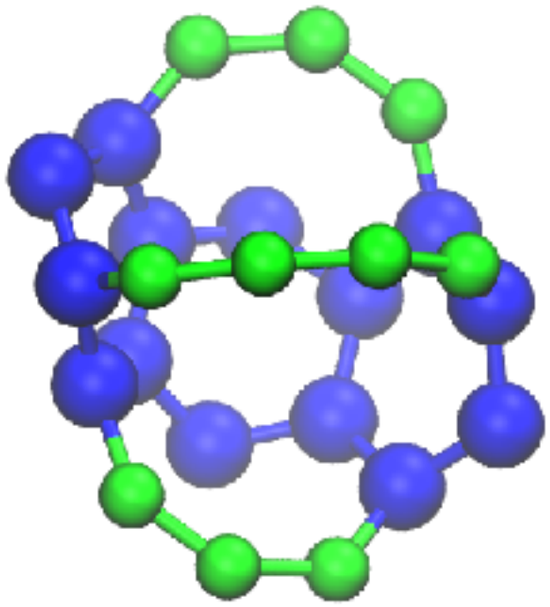
E = 0.06 eV/atoms



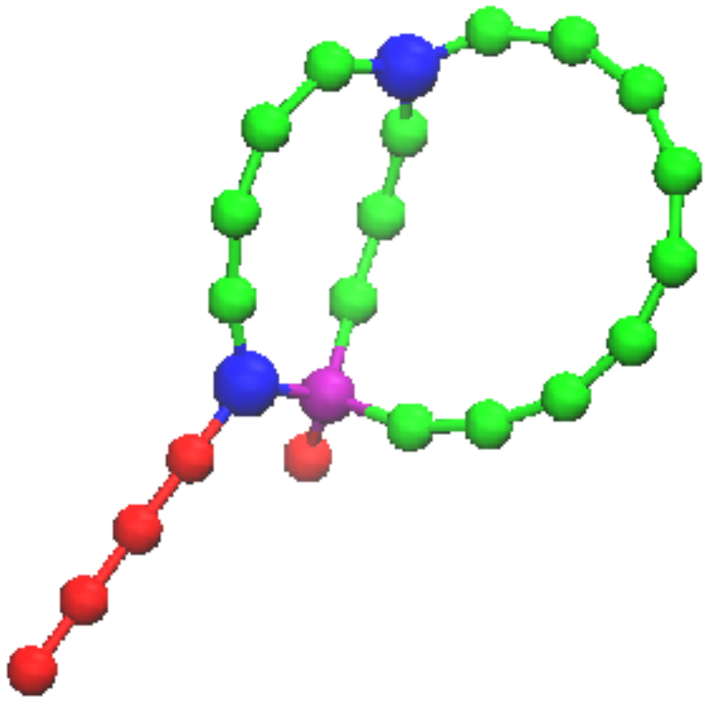
E = 0.17 eV/atoms



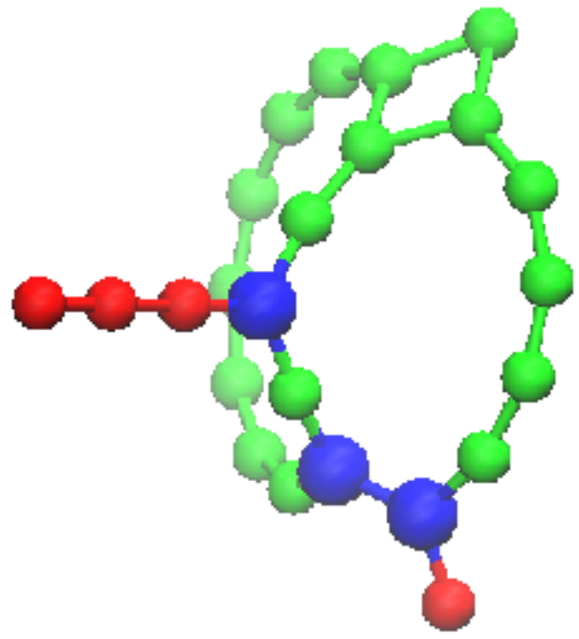
E = 0.18 eV/atoms



E = 0.48 eV/atoms



E = 0.48 eV/atoms



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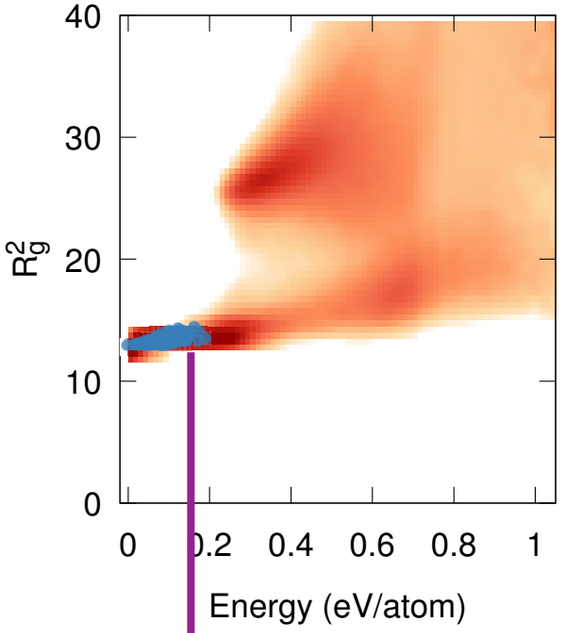
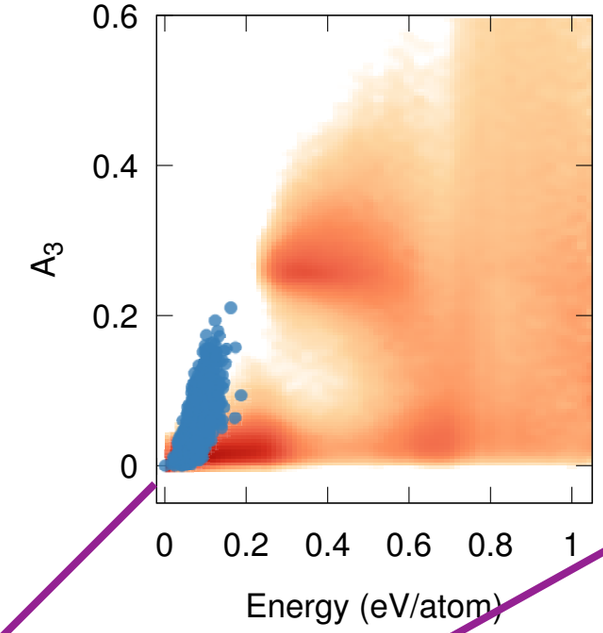
Analysis of the quenched structure: C_{60}

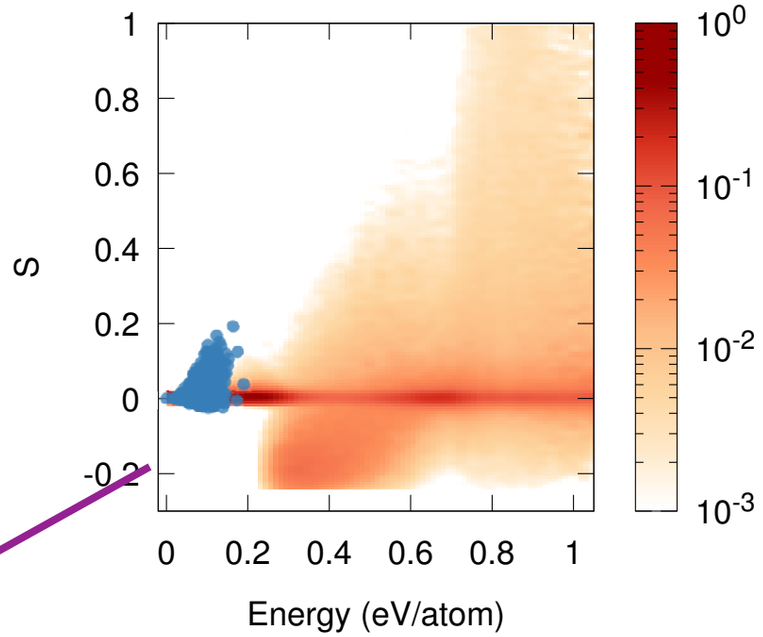
squared radius of gyration

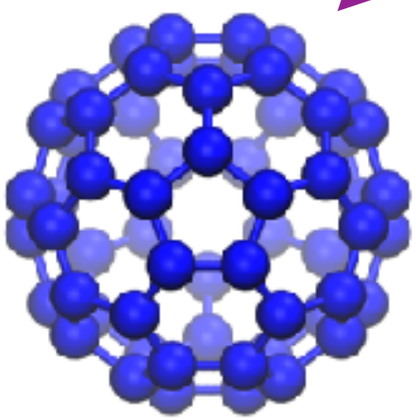


asphericity

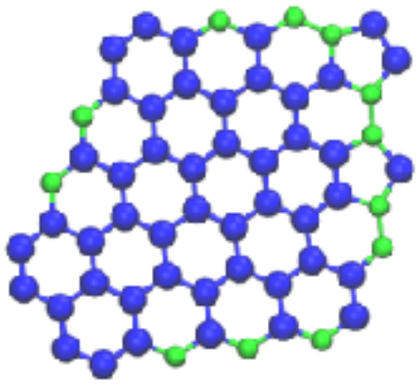


prolateness





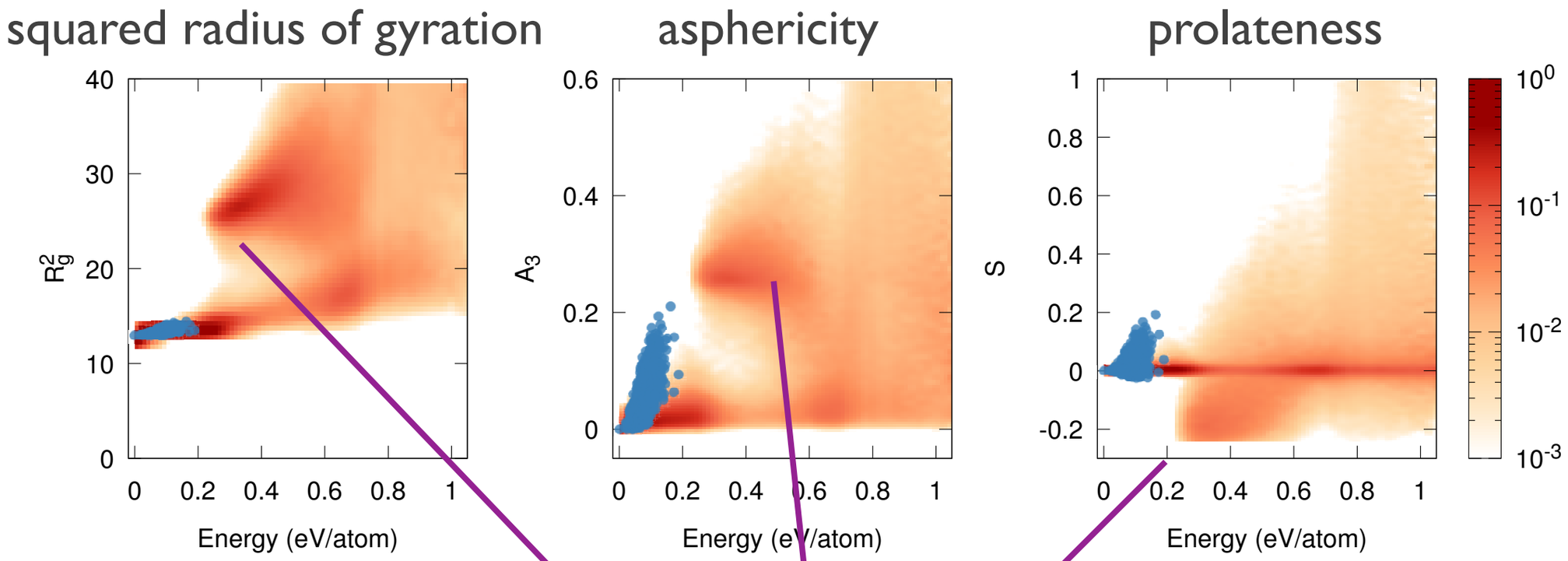
Fullerene isomers (1812)

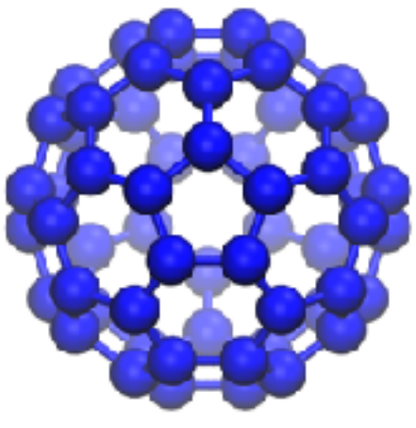


planar hexagonal

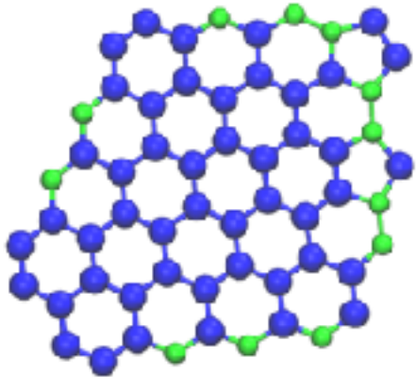
LAMMPS

Analysis of the quenched structure: C_{60}





Fullerene isomers (1812)

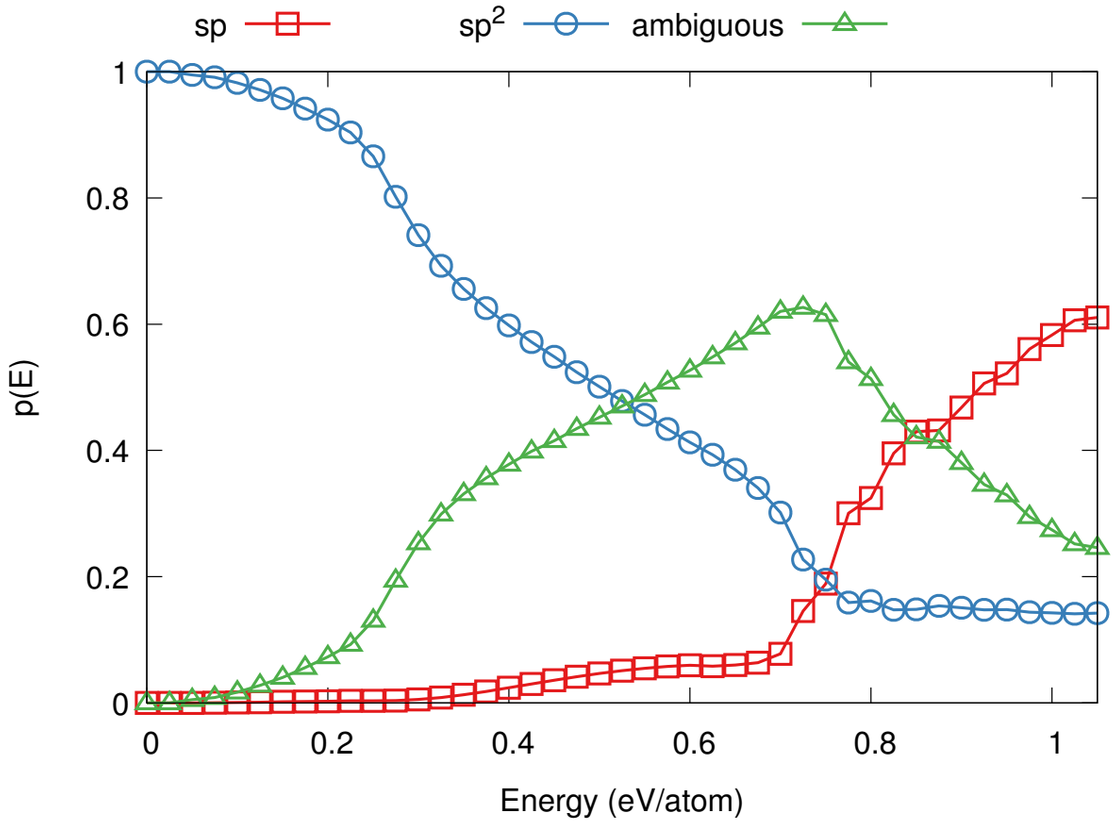


planar hexagonal

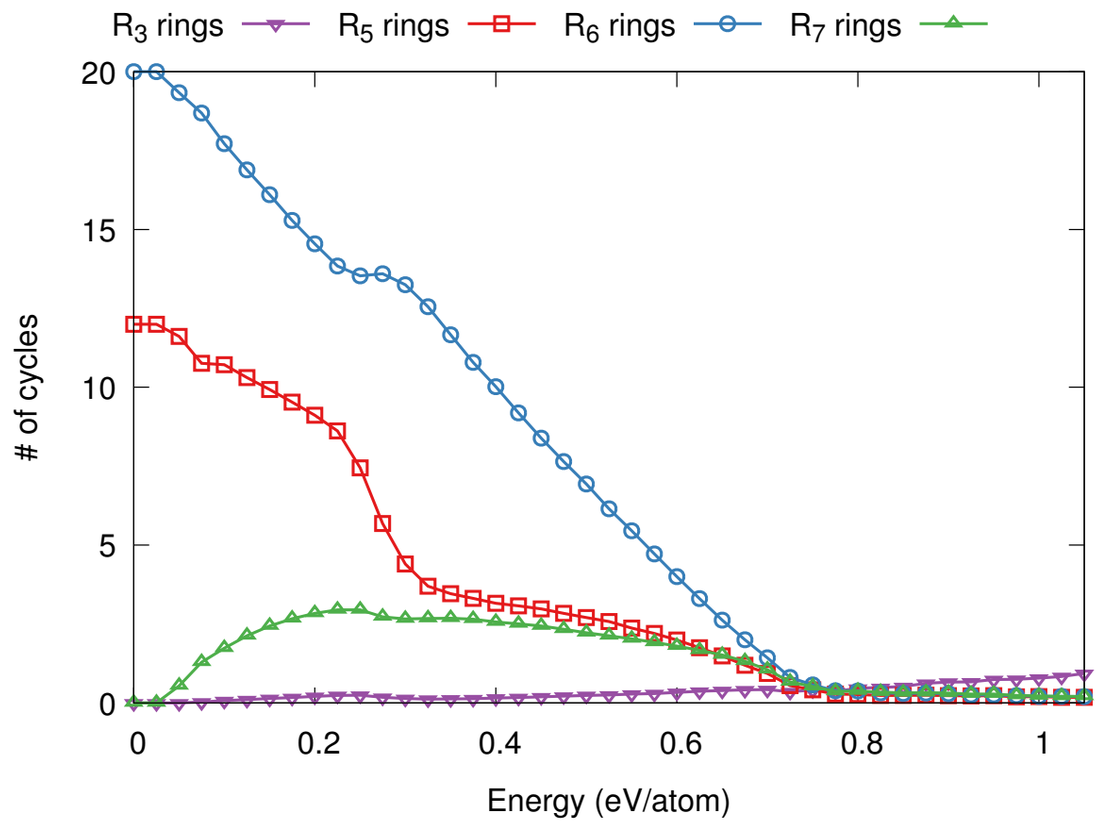
LAMMPS

C_{60}

hybridization state



of cycles



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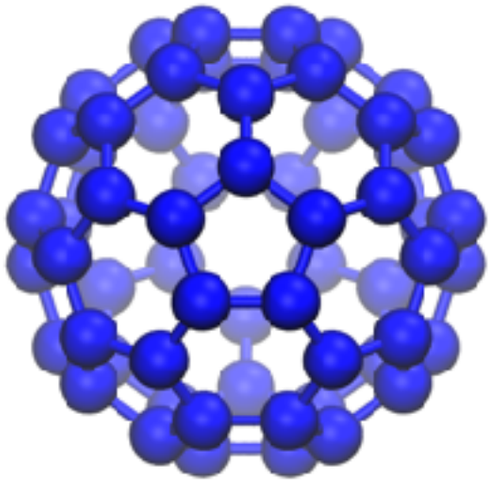
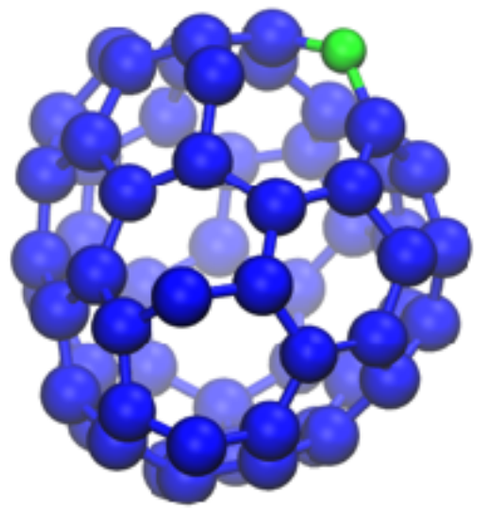
Analysis of the quenched structures: C_{60}

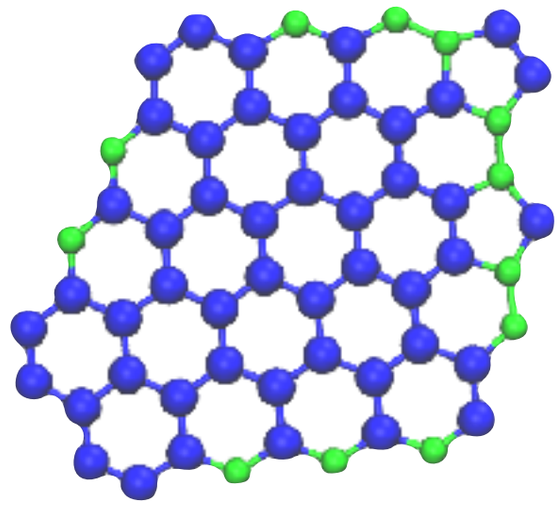
E = 0



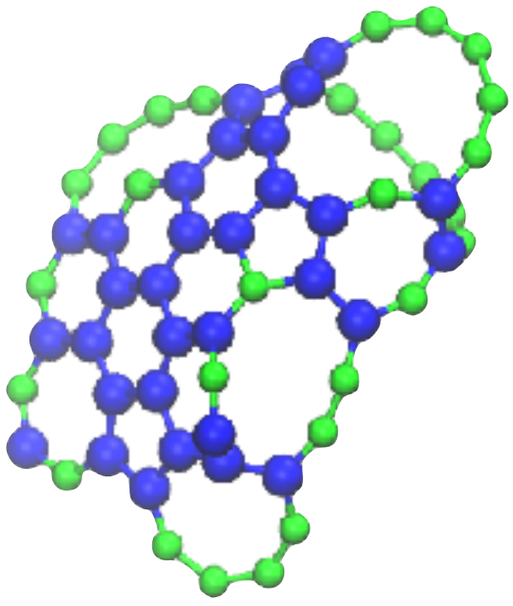
E = 0.12 eV/atoms



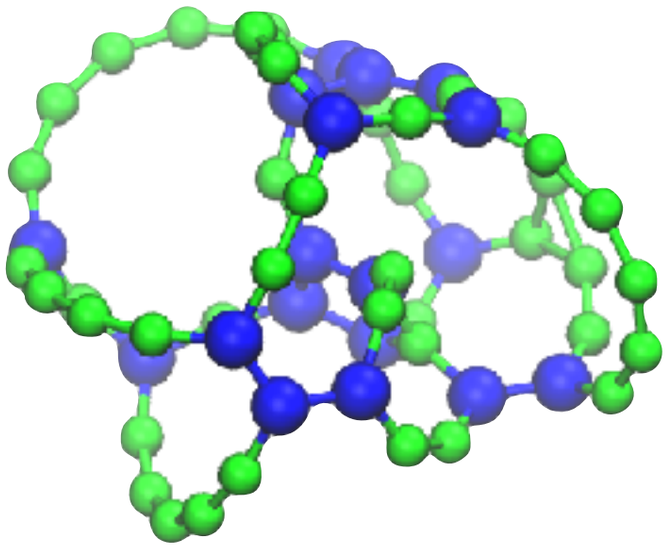
E = 0.24 eV/atoms



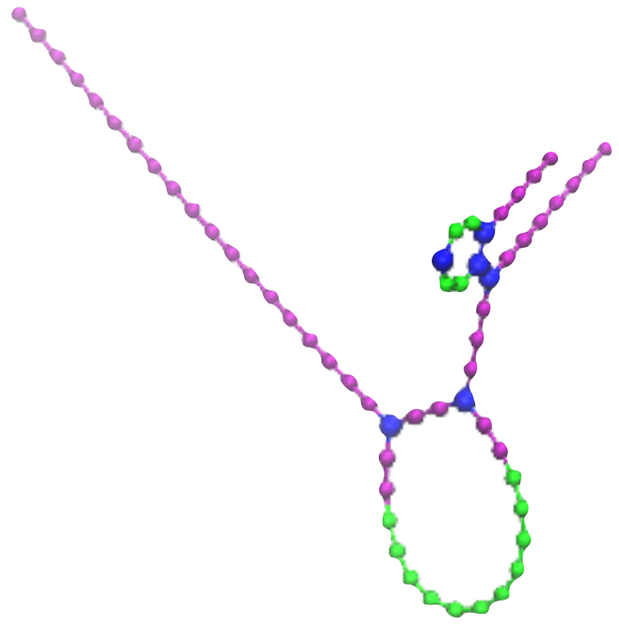
E = 0.48 eV/atoms



E = 0.72 eV/atoms



E = 0.88 eV/atoms



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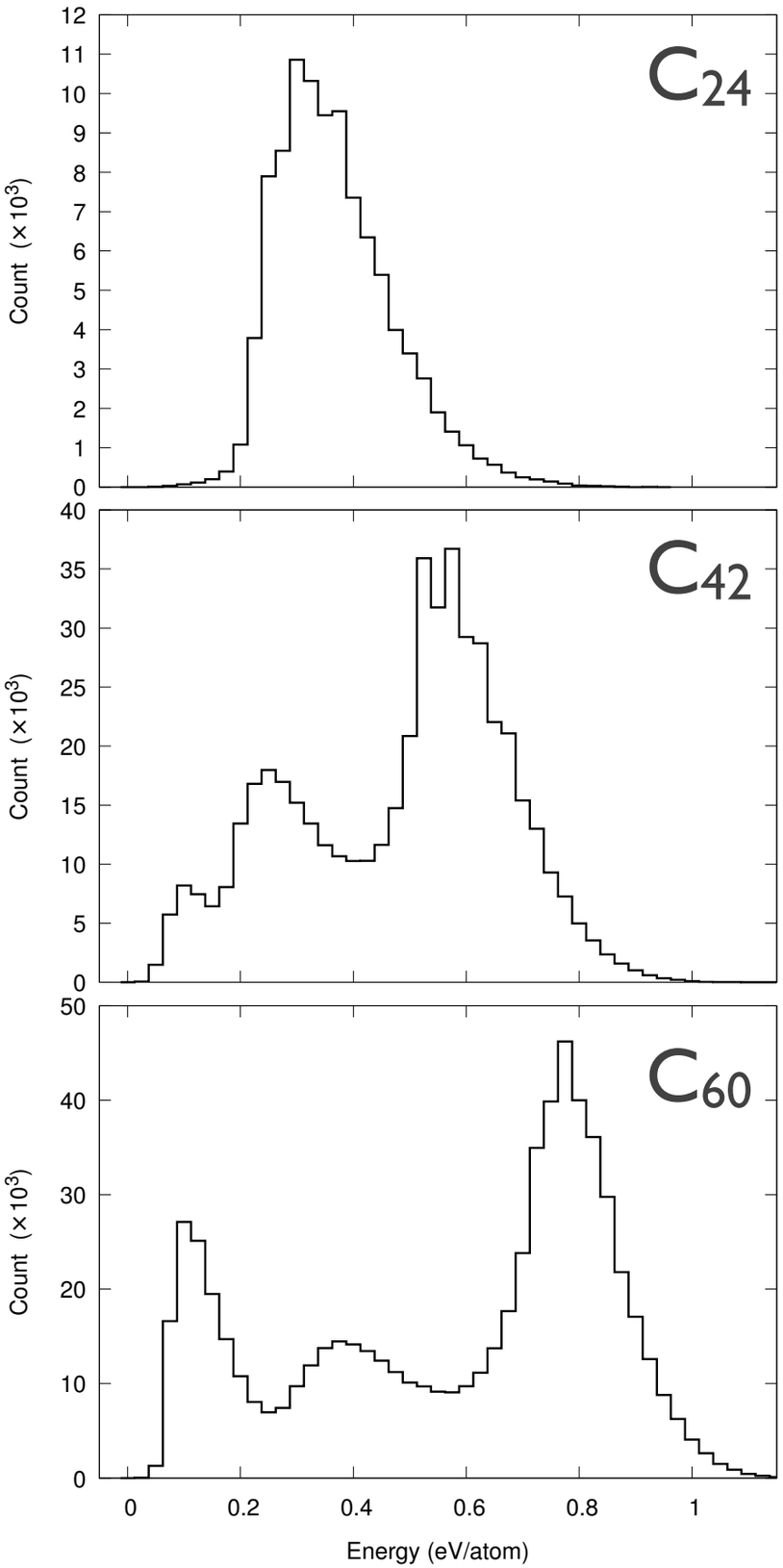
Conclusions

- LAMMPS is a power MD tool for simulate the structuration of carbon clusters
- The current implementation of (AI)REBO in LAMMPS is bug free
- AIREBO is not a derivable potential
- Some parameters in REBO need to be changed (this can be easily fixed)

THANKS FOR YOUR ATTENTION

Energy distribution of quenched structures



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Local structural analysis

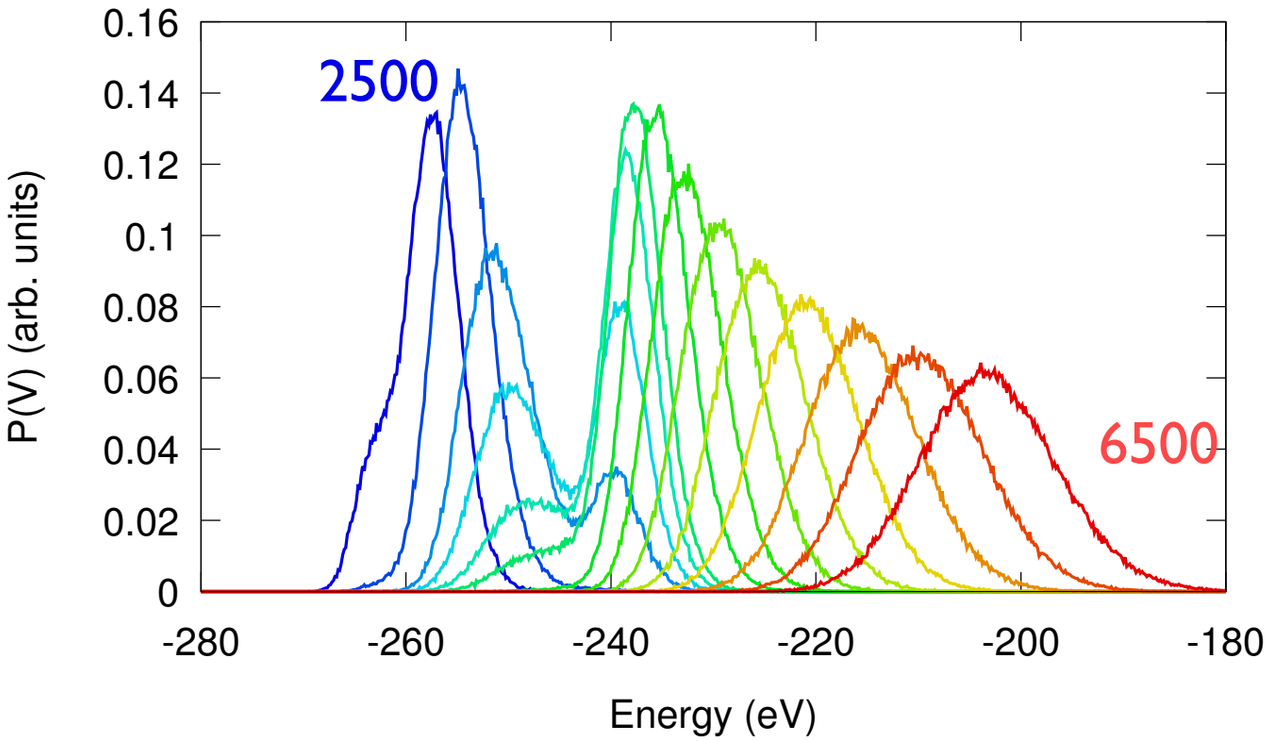
- Hybridization state: purely geometrical definition from the number of neighbors and the angles

$$\text{sp}: \begin{cases} N(i) = 1 \text{ or } 2, \\ \theta_k > 170^\circ \ \forall \ k. \end{cases}$$

$$\text{sp}^2: \begin{cases} N(i) = 2 \text{ or } 3, \\ 100^\circ < \theta_k < 125^\circ \ \forall \ k, \\ \text{Var}(\theta_k) < 12^\circ. \end{cases}$$

$$\text{sp}^3: \begin{cases} N(i) = 4, \\ 100^\circ < \theta_k < 120^\circ \ \forall \ k, \\ \text{Var}(\theta_k) < 12^\circ. \end{cases}$$

C_{42}: exemple of REMD simulation



ρ=0.15 g/cm³, R=11 Å

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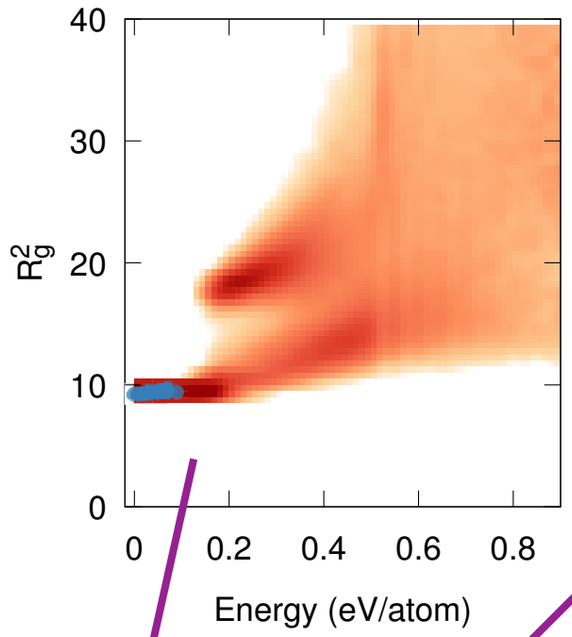
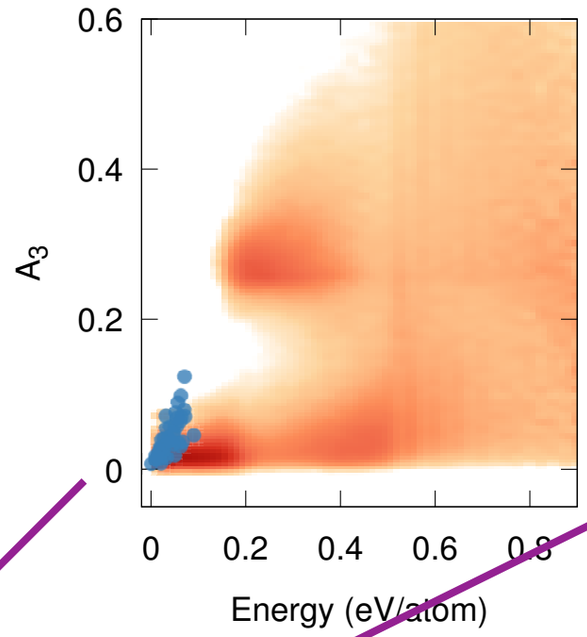
Analysis of the quenched structure: C_{42}

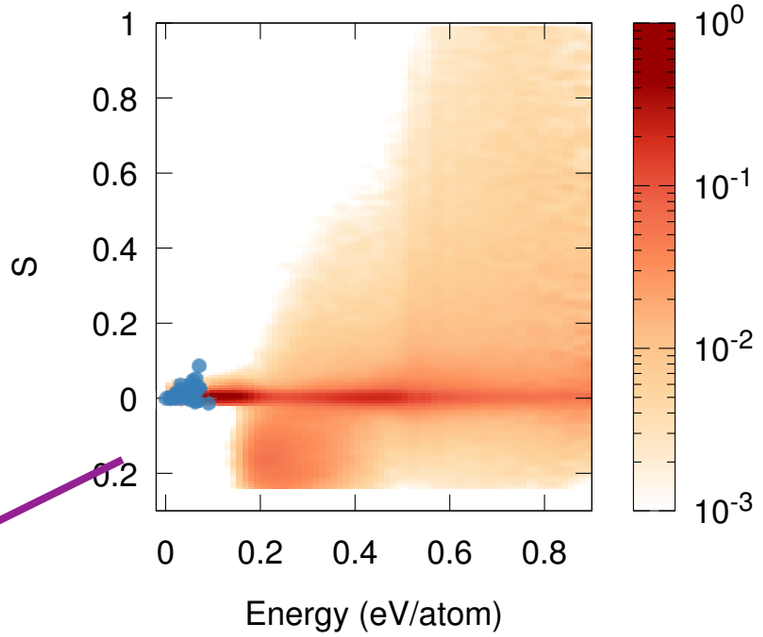
squared radius of gyration

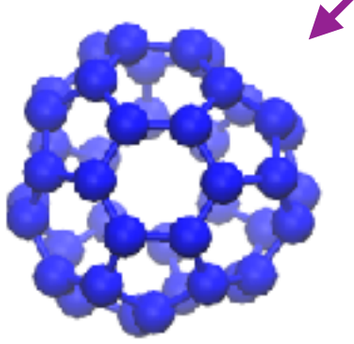


asphericity



prolateness





45 fullerene isomers

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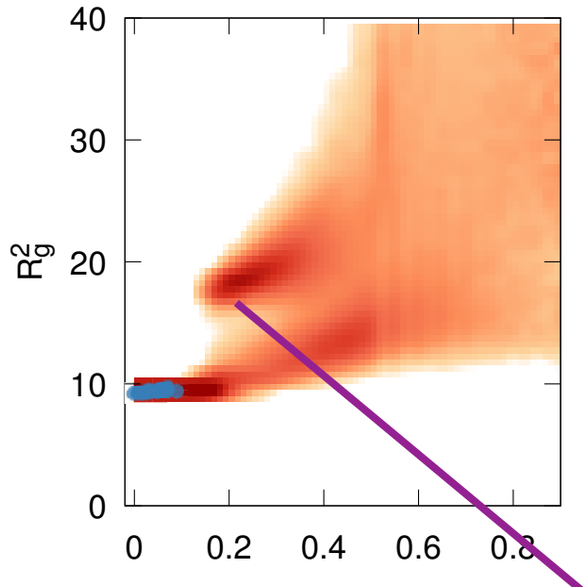
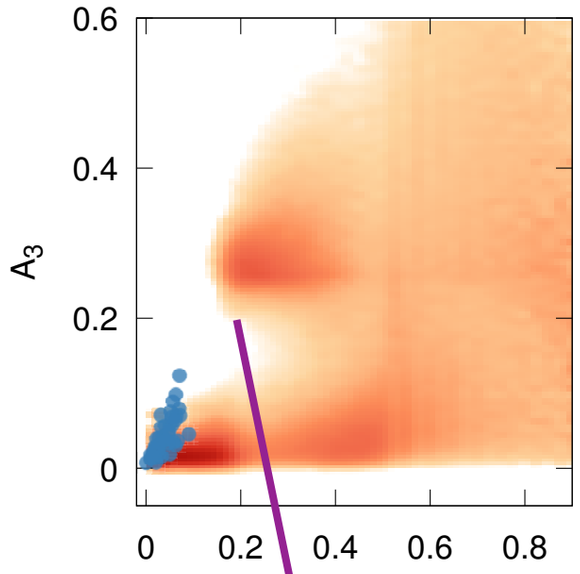
Analysis of the quenched structure: C_{42}

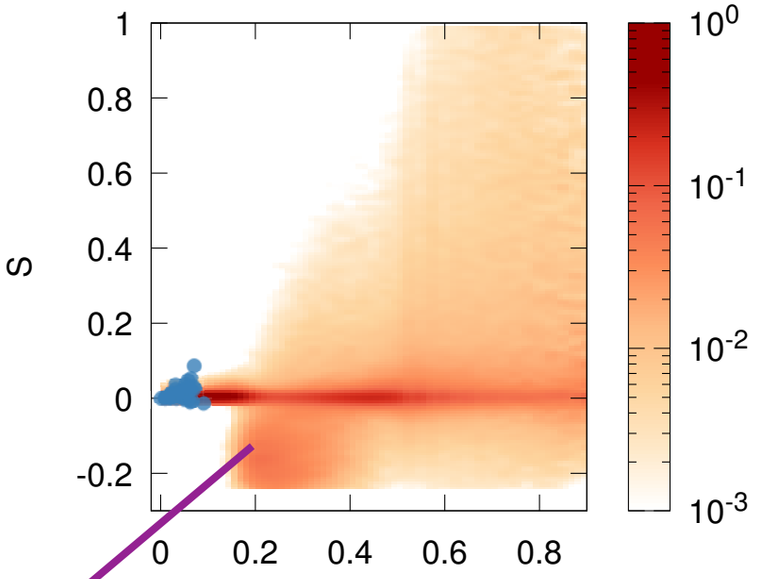
squared radius of gyration

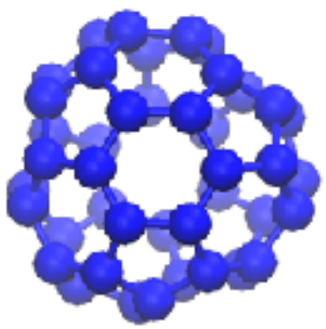


asphericity

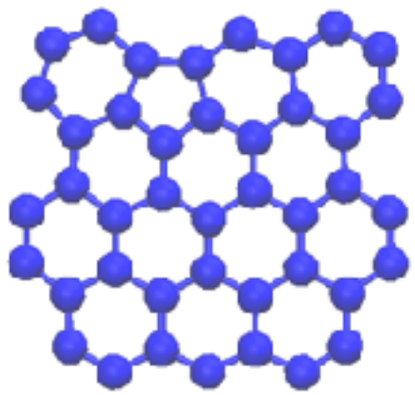


prolateness





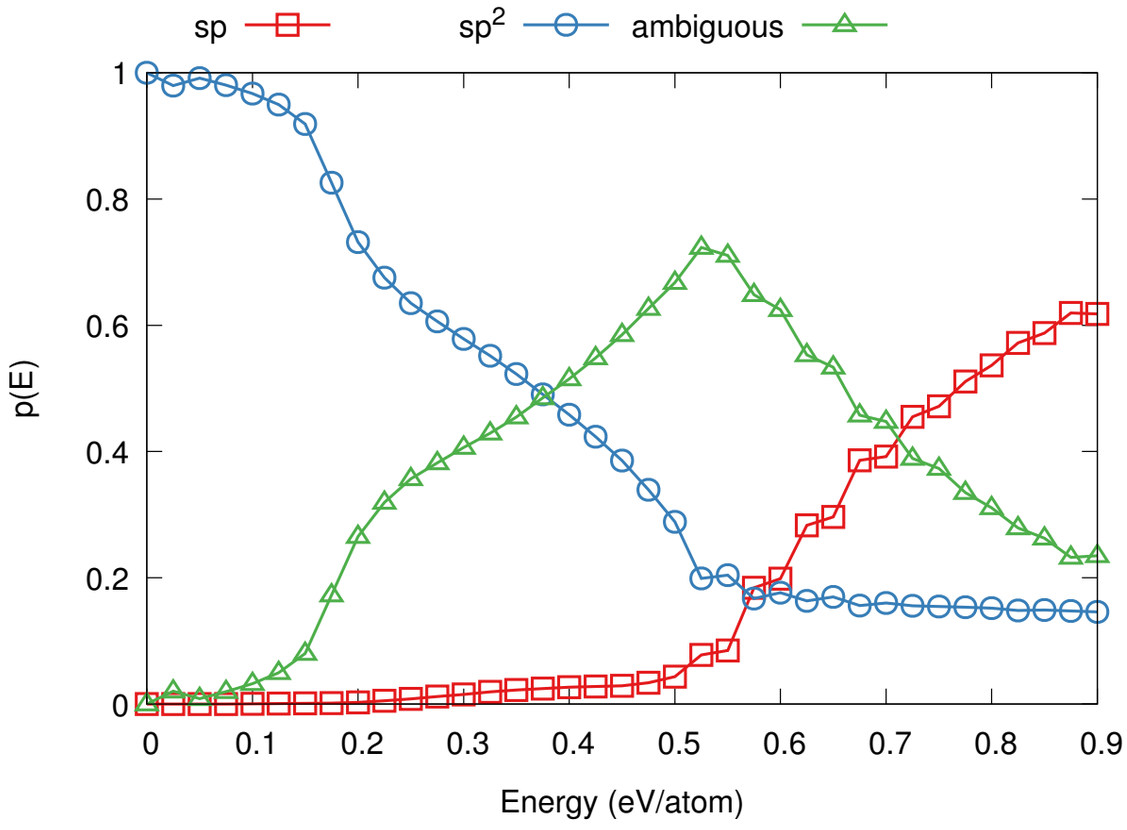
45 fullerene isomers

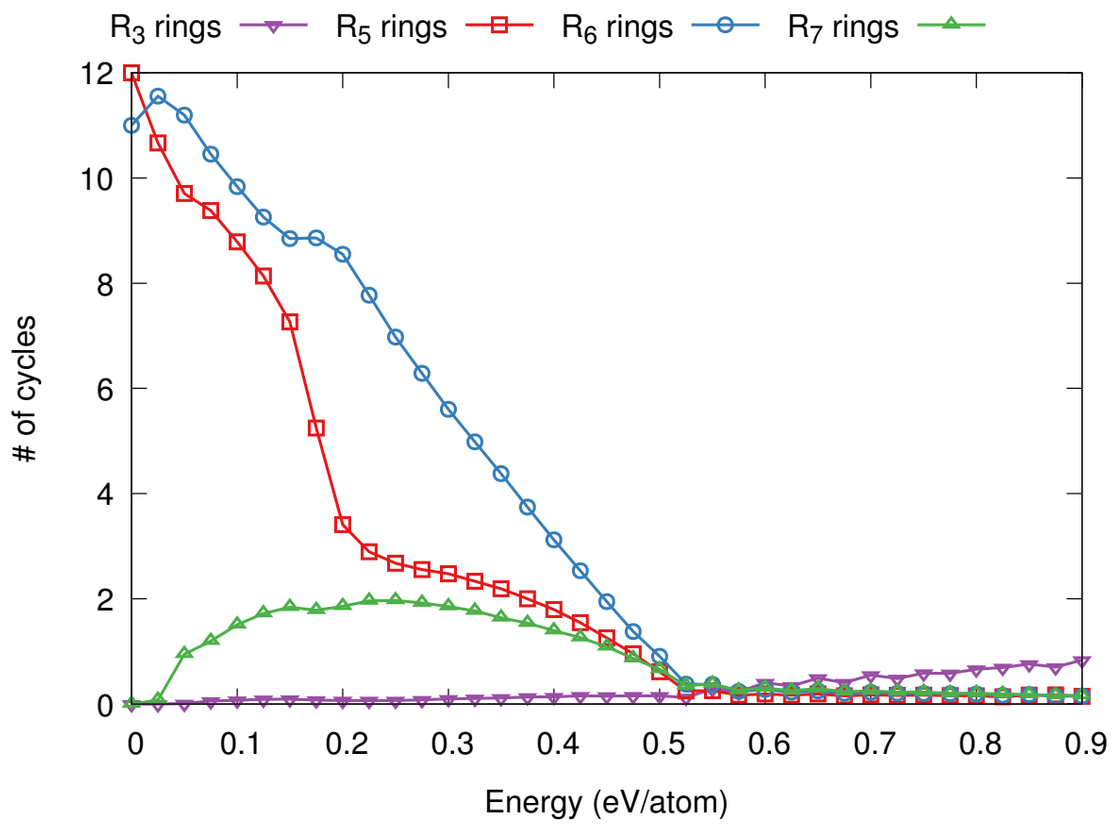


planar structures

LAMMPS

Analysis of the quenched structure: C_{42}





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