
Modeling the Sputtering of Amorphous Carbon with Bond- Order Potentials

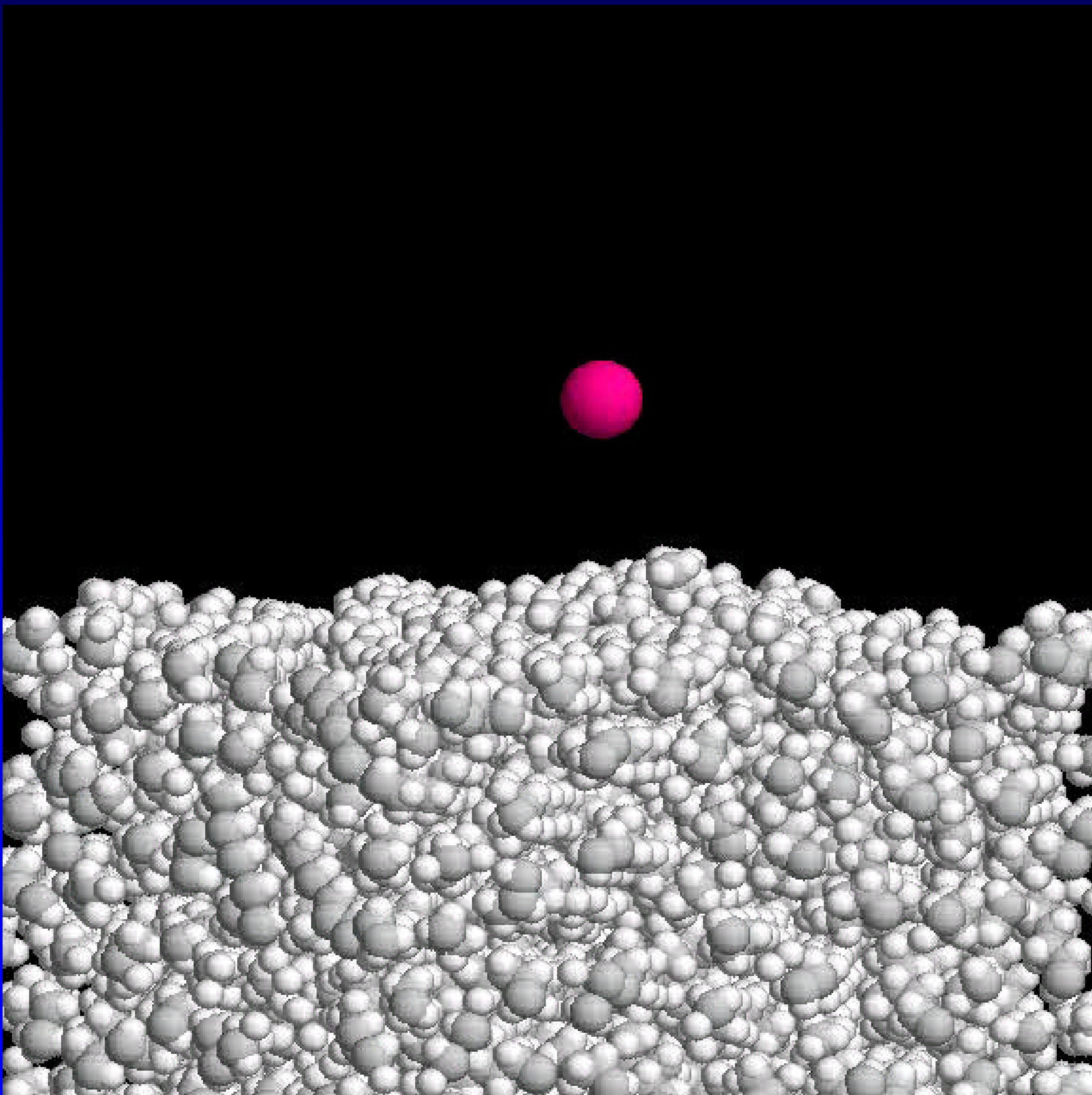
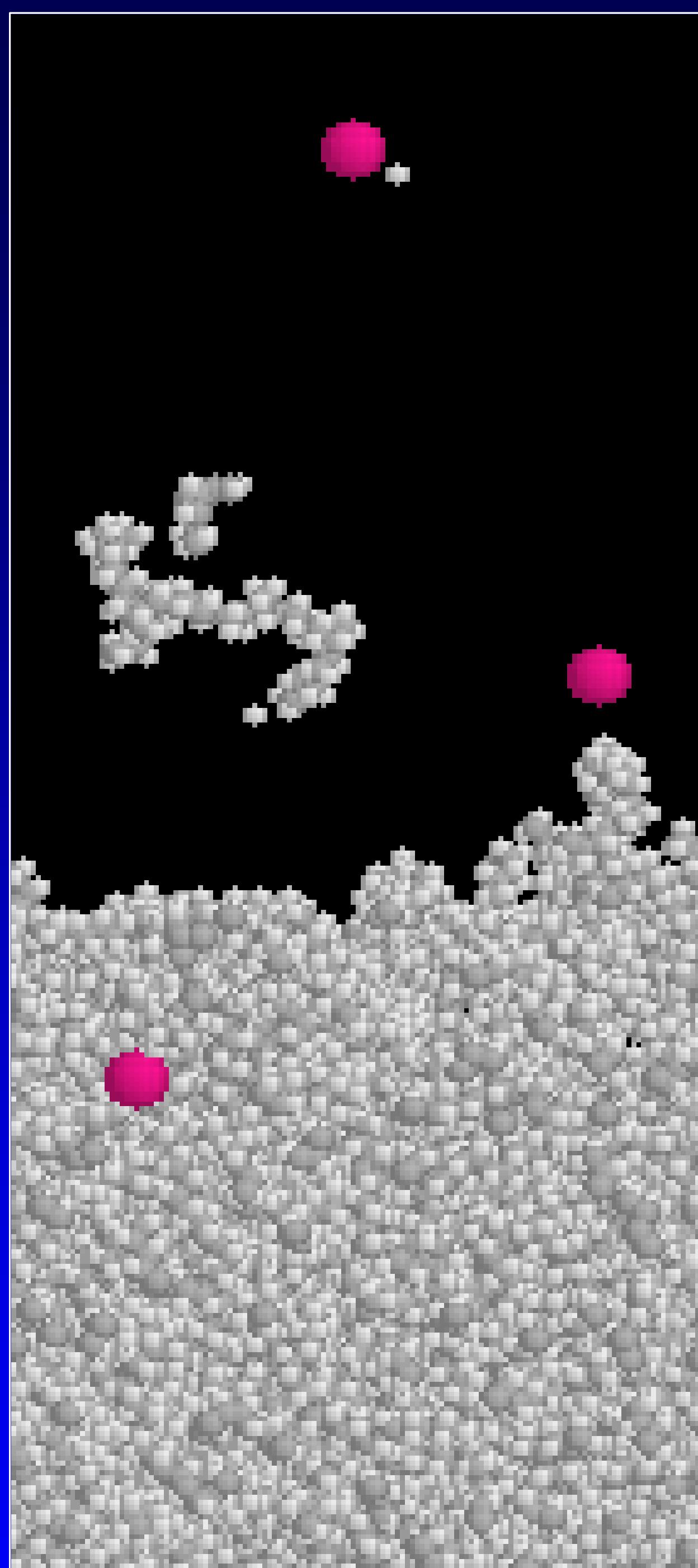
Steven J. Stuart



PSIF Workshop
ORNL

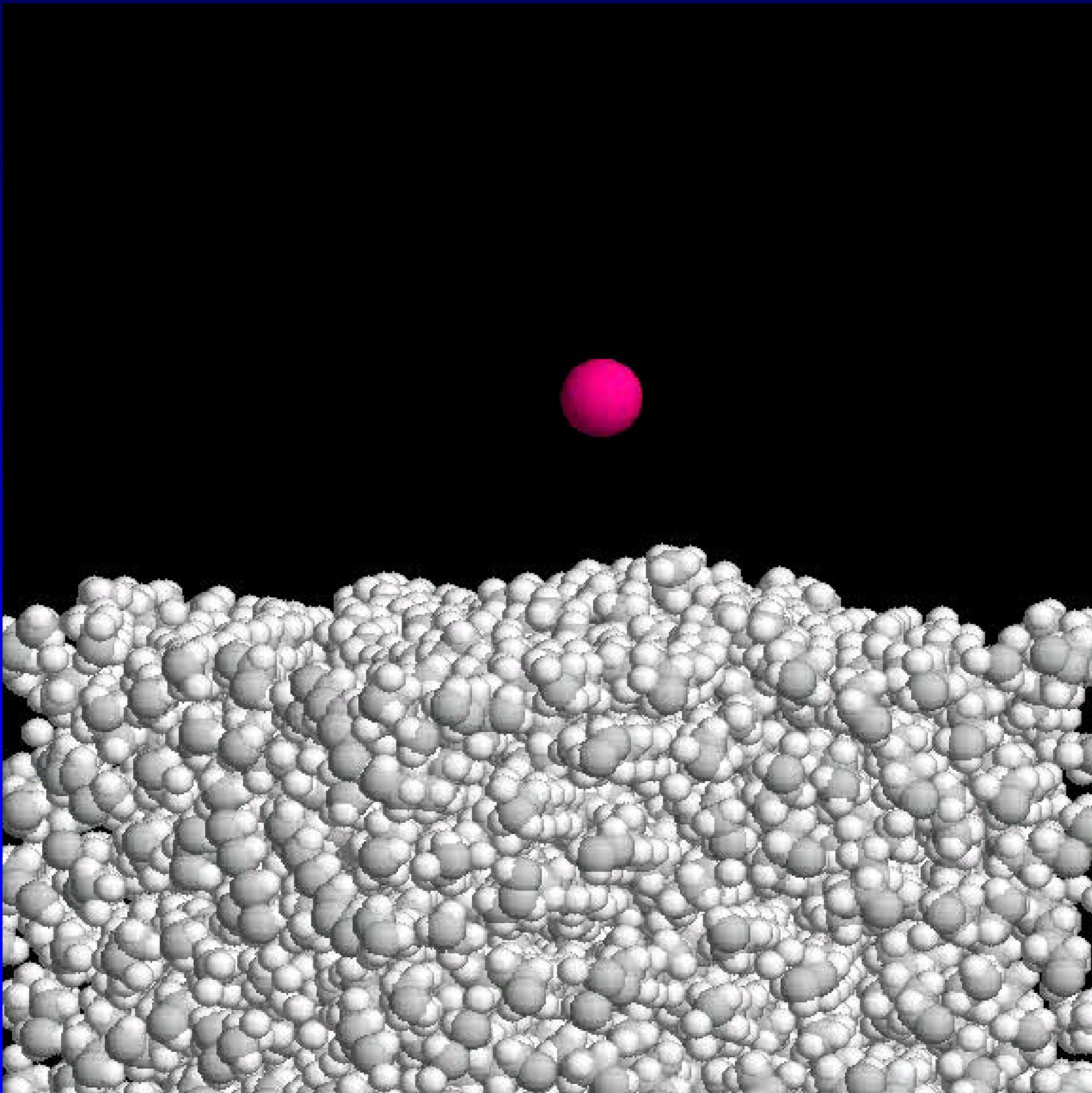
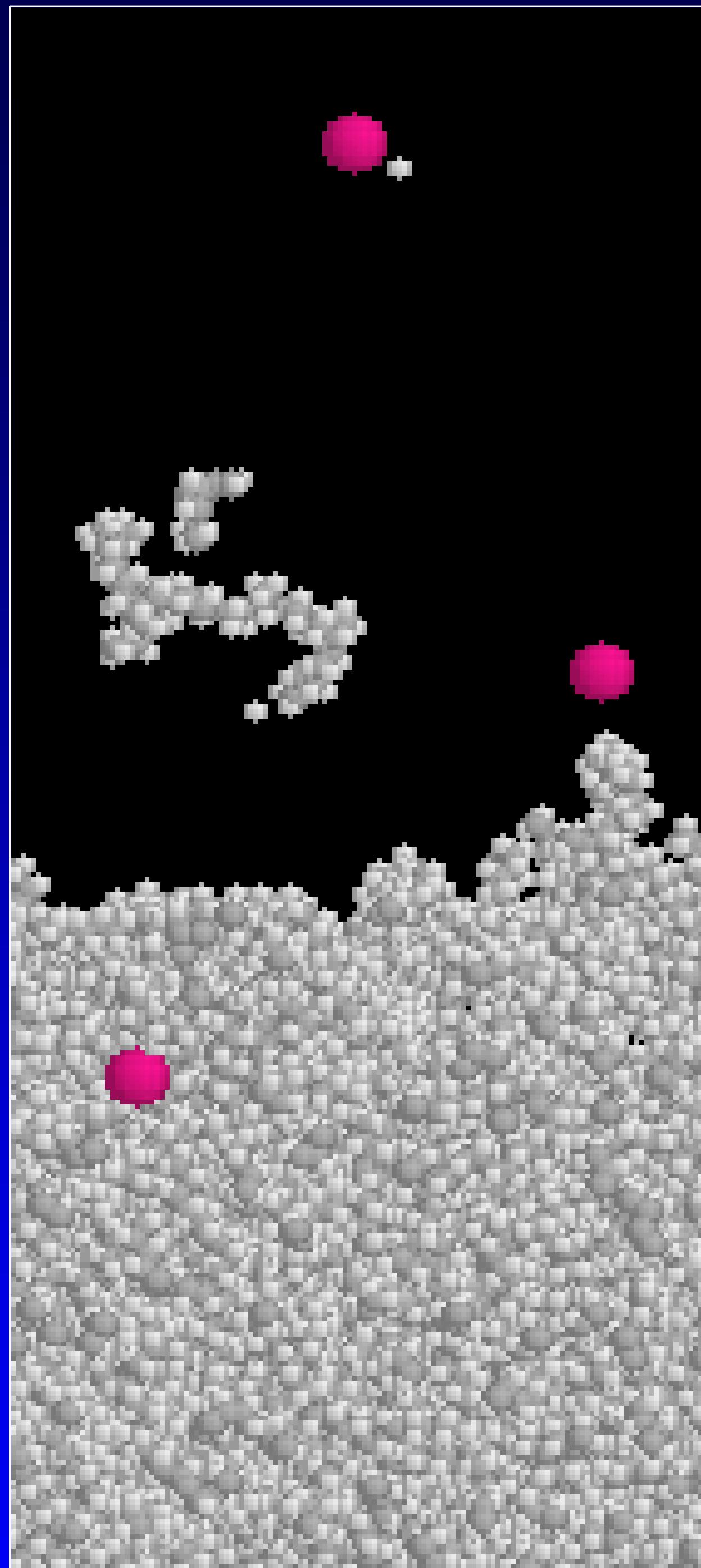
March 23, 2005

Sputtering of Soft Materials



- Krstic movie
- 500 eV impact
- Ar ? supersaturated a-C:H

Sputtering of Soft Materials



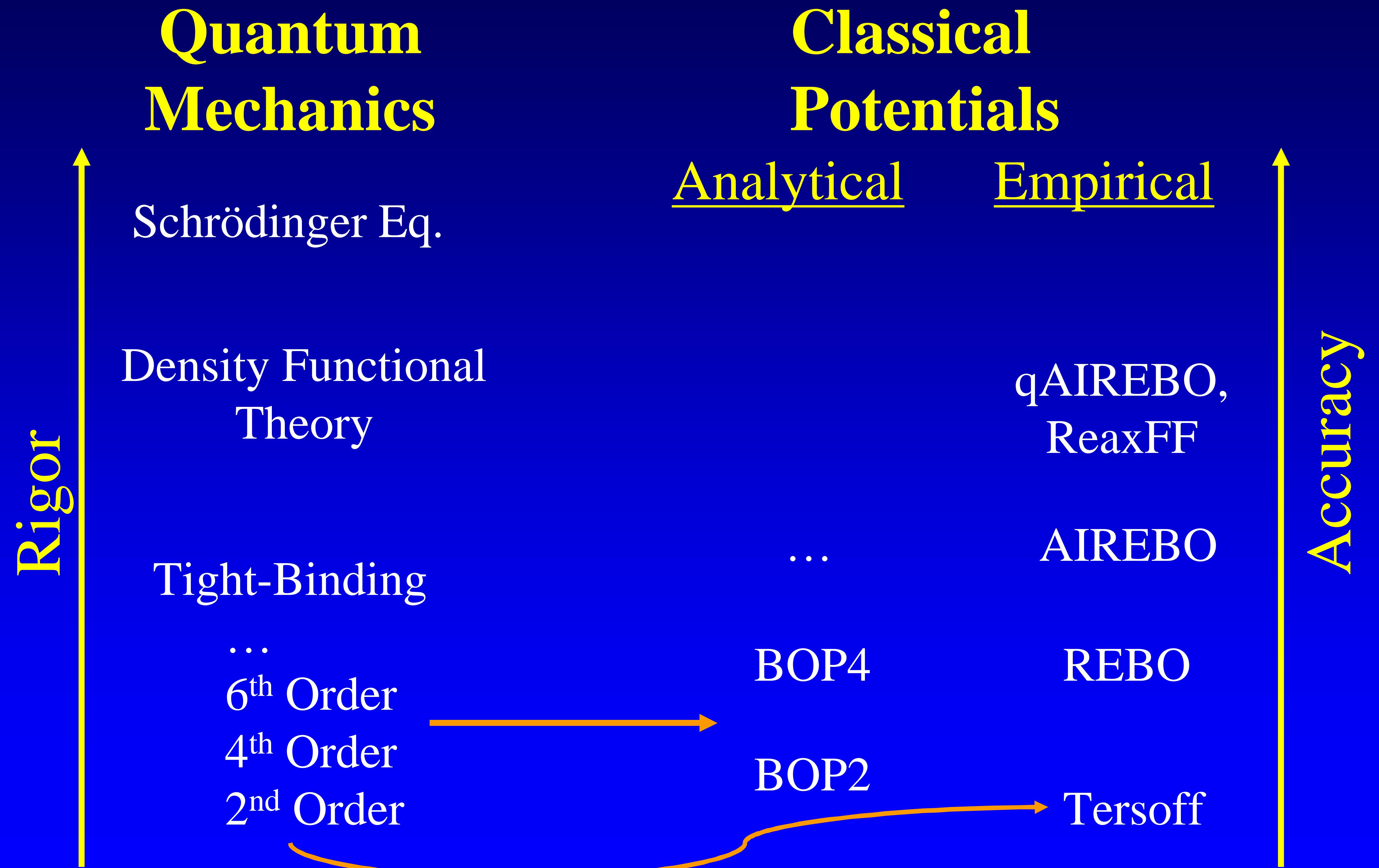
- Krstic movie
- 500 eV impact
- Ar ? ~~supersaturated a C:H-~~ Branched polyethylene

Motivation

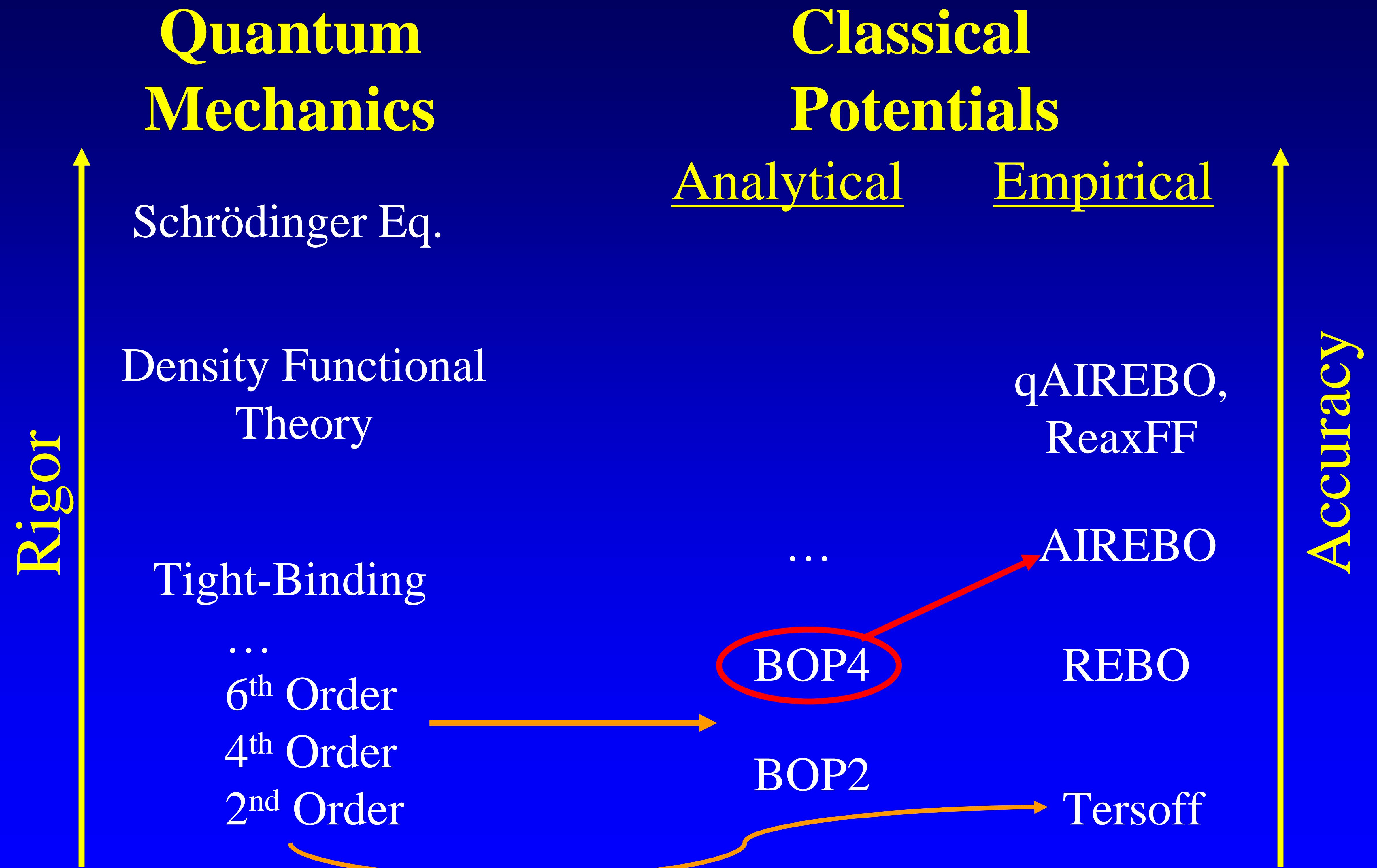
Preliminary studies with an eye towards:

- Potential development
- Input to coarse-grained MC models
 - Reflection
 - Particle creation
 - Diffusivities
- Investigate accelerated dynamics methods
 - ps ? μ s ? ms?
 - Parallel replica dynamics, hyperdynamics, TAD

Classes of Models



Classes of Models



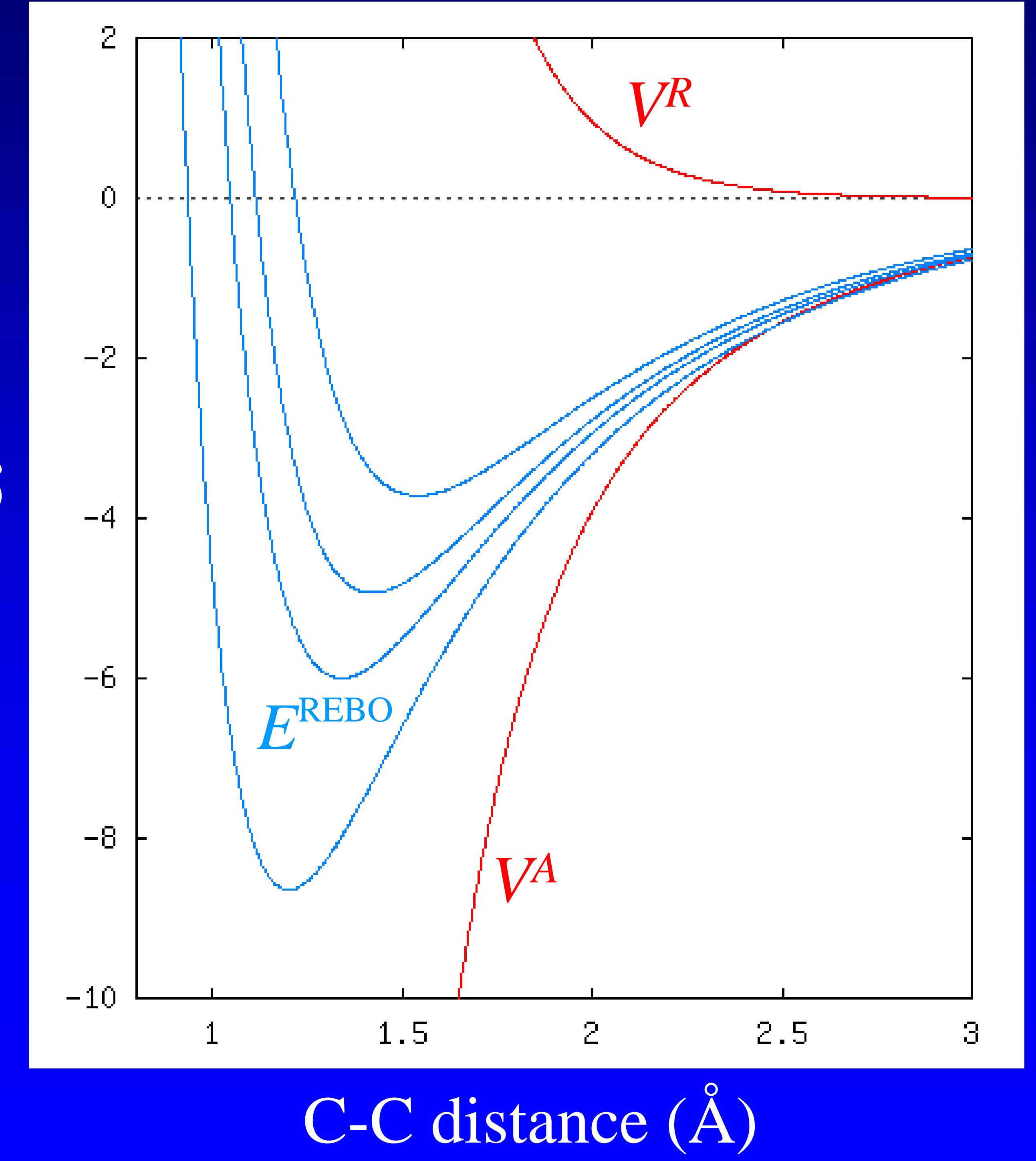
REBO Potential

(Reactive Empirical Bond Order)

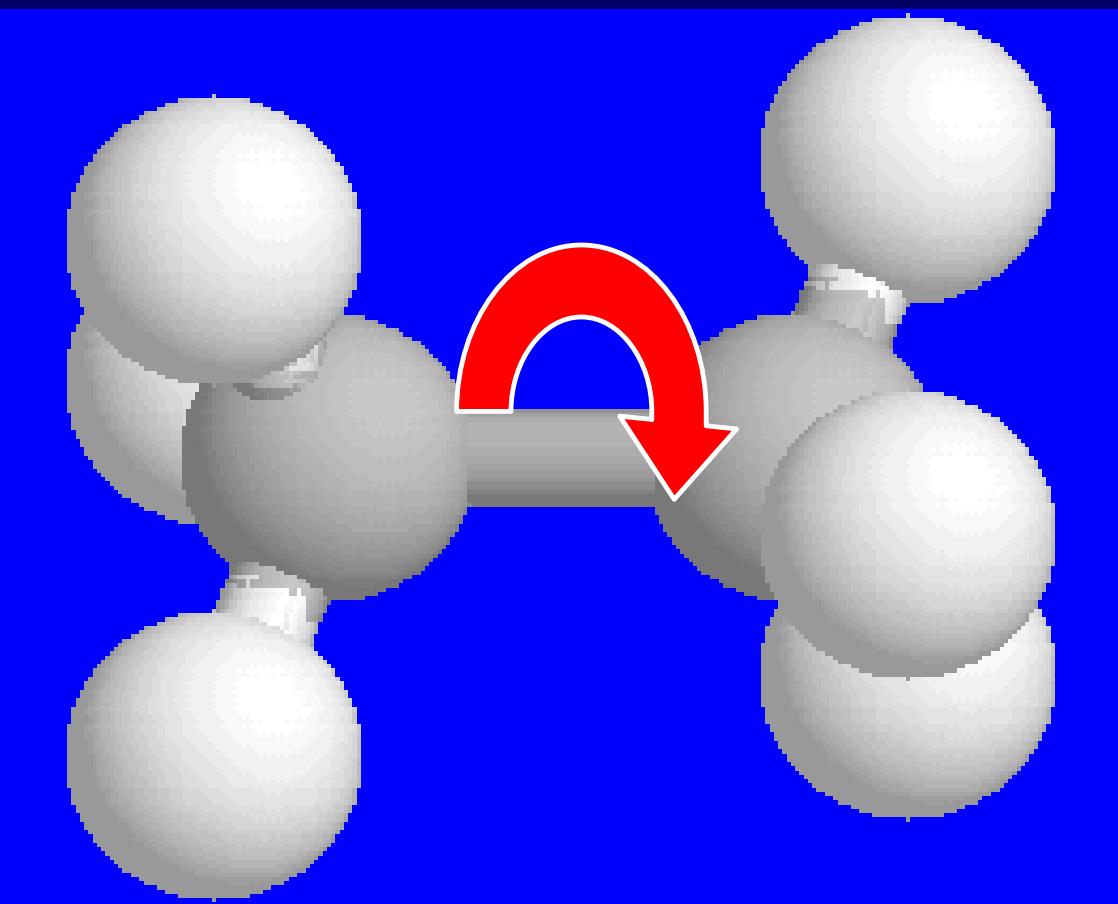
$$V_{ij}^{\text{REBO}} = V_{ij}^R + b_{ij} V_{ij}^A$$

$$V_{ij}^R = \left(1 + \frac{Q_{ij}}{r_{ij}} \right) A_{ij} e^{-\mathbf{a}_{ij} r_{ij}}$$

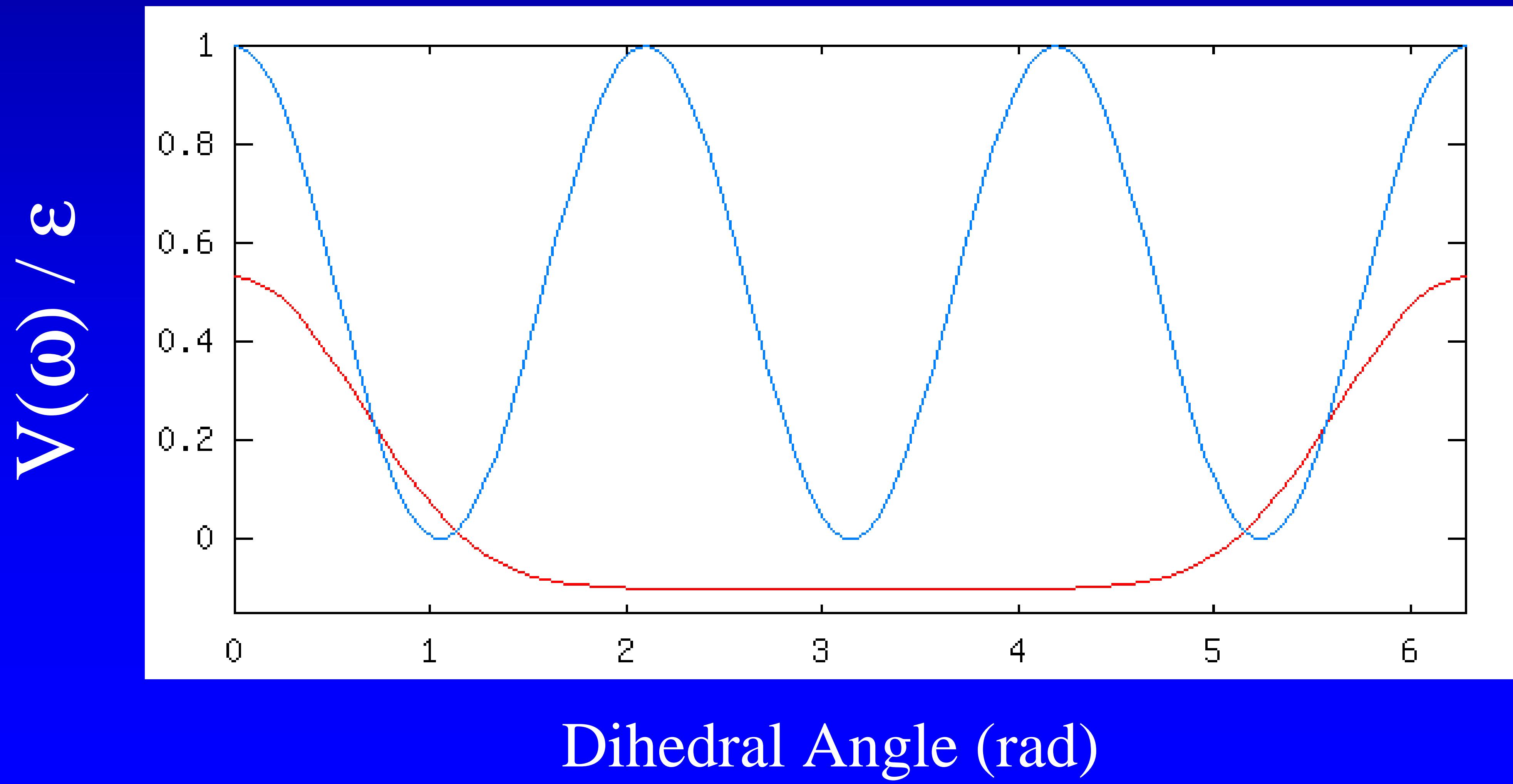
$$V_{ij}^A = \sum_{n=1}^3 B_{ij}^{(n)} e^{-\mathbf{b}_{ij}^{(n)} r_{ij}}$$



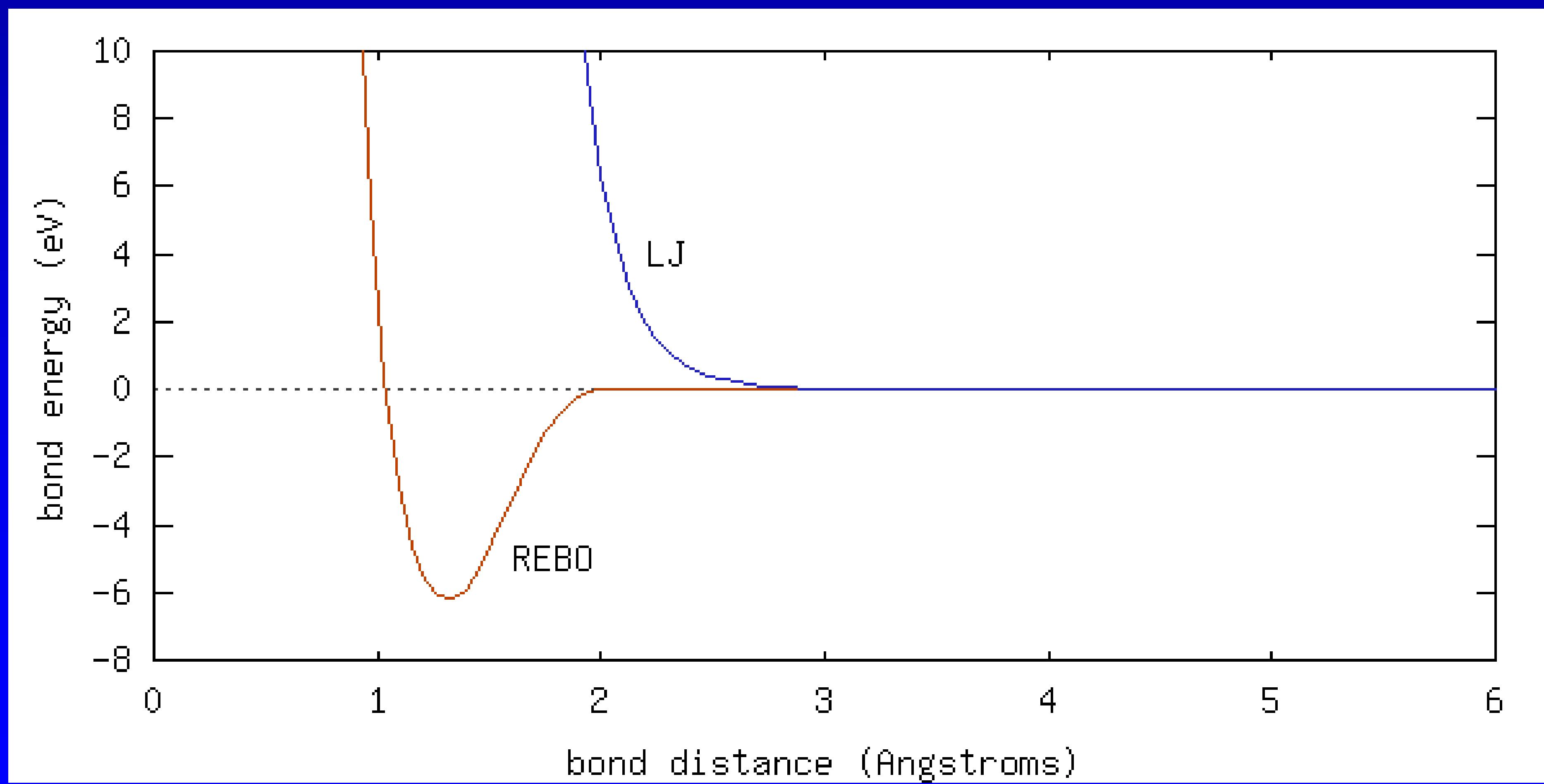
AIREBO Torsional Potential



$$V(w) = e \left[\frac{256}{405} \cos^{10} \frac{w}{2} - \frac{1}{10} \right]$$

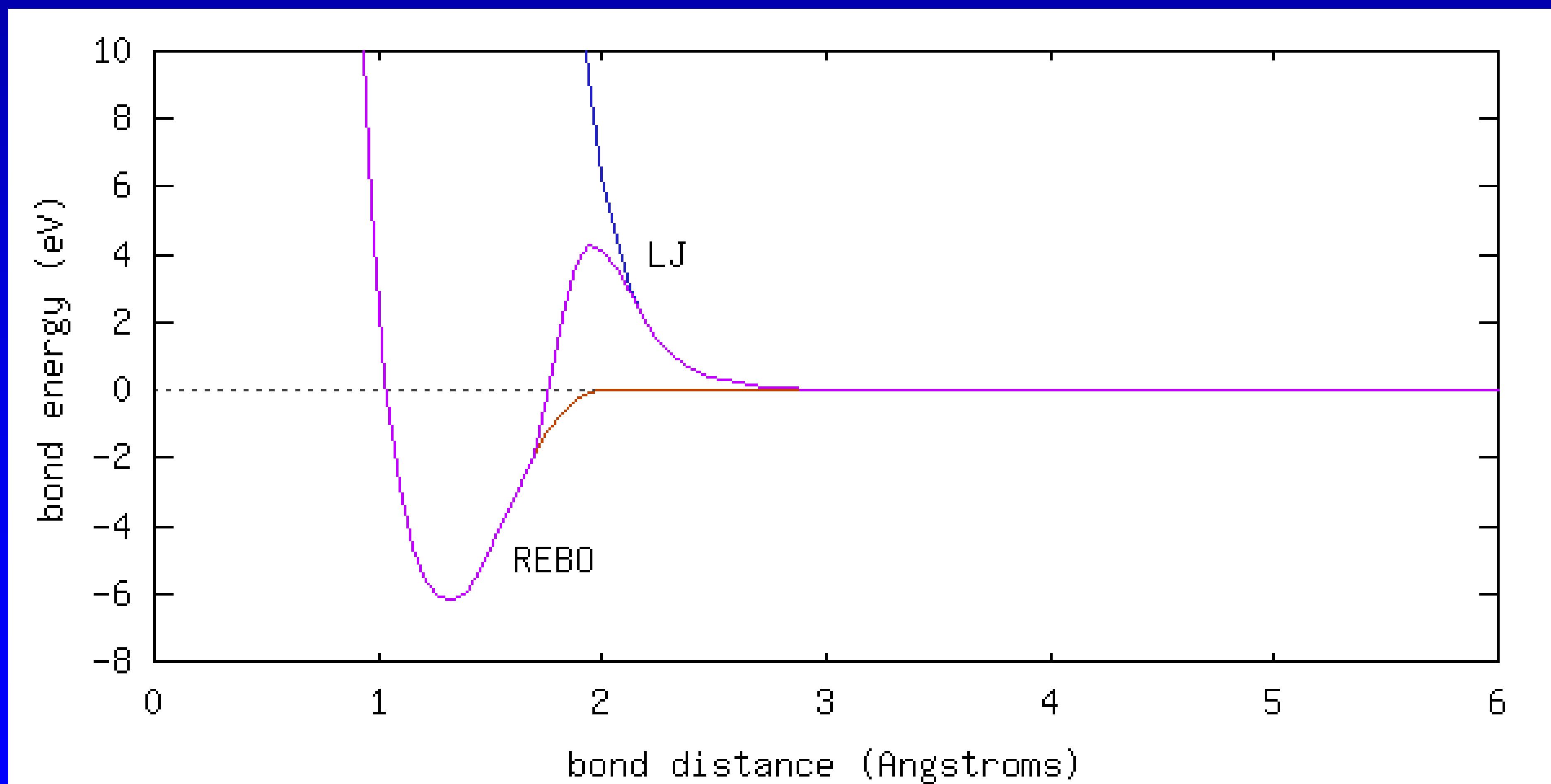


AIREBO Nonbonded Potential



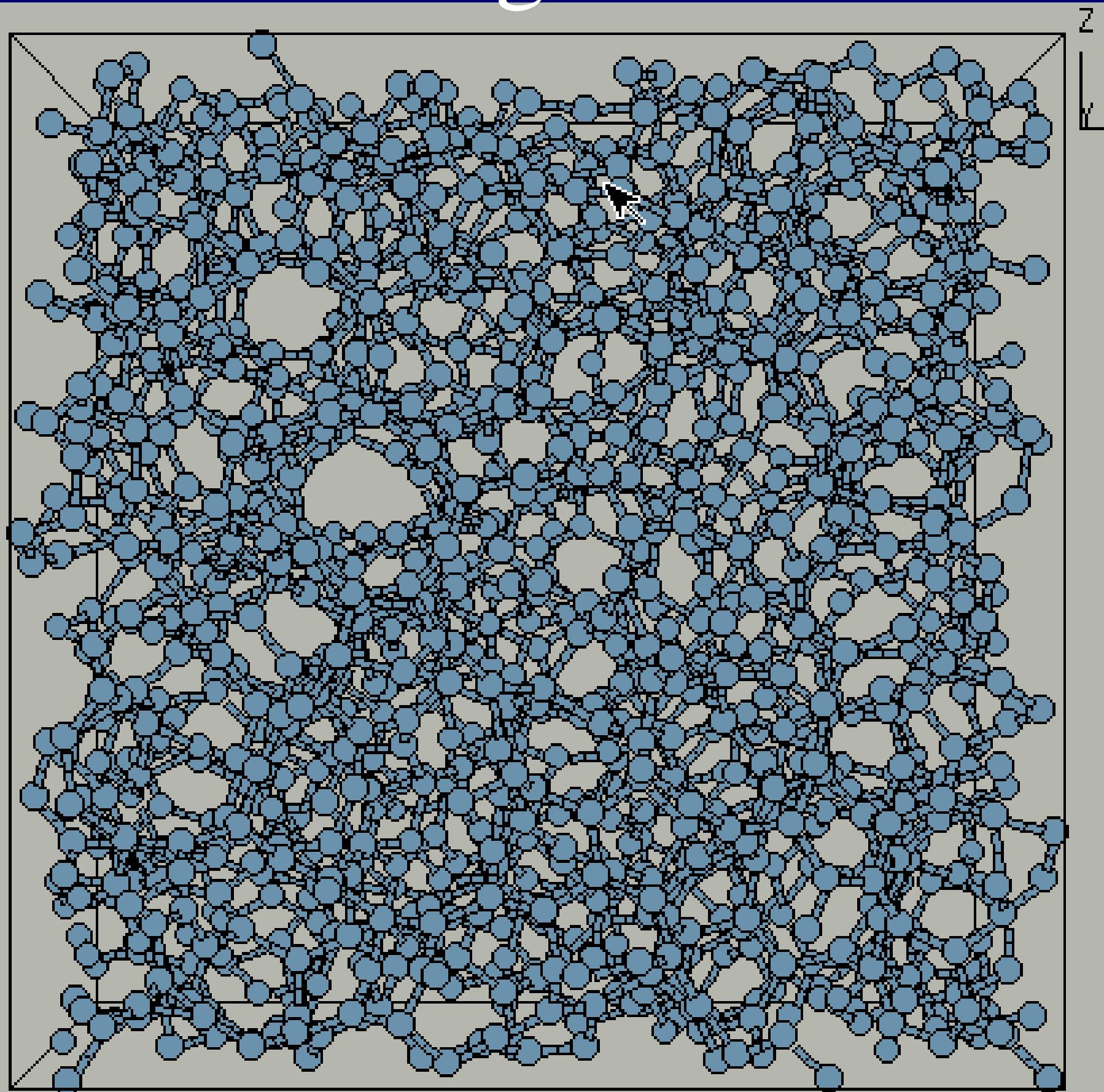
AIREBO Nonbonded Potential

$$V(r) = S(r)S'(b)CV^{\text{LJ}}(r) + [1 - S(r)]CV^{\text{LJ}}(r)$$

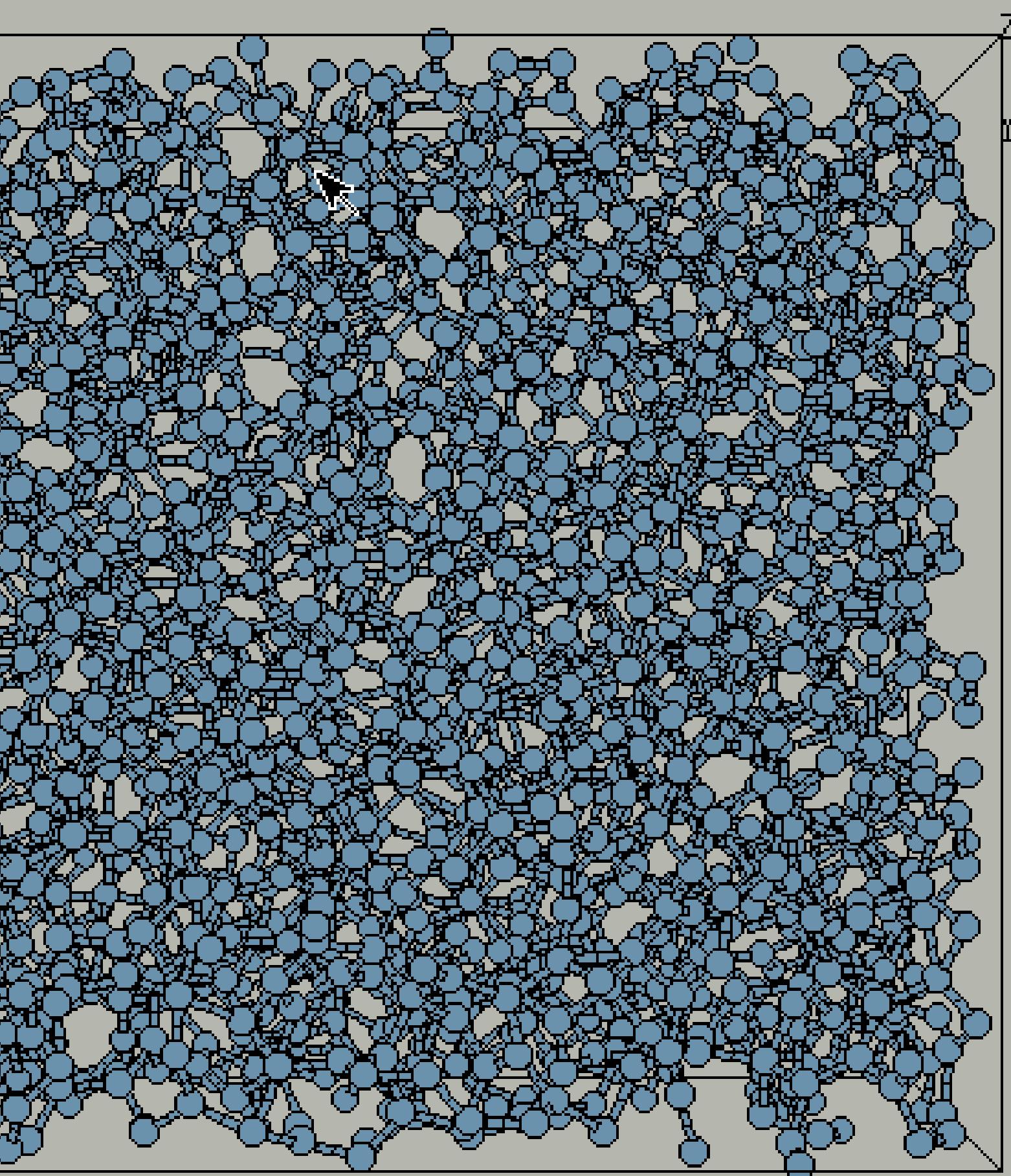


Amorphous Carbon

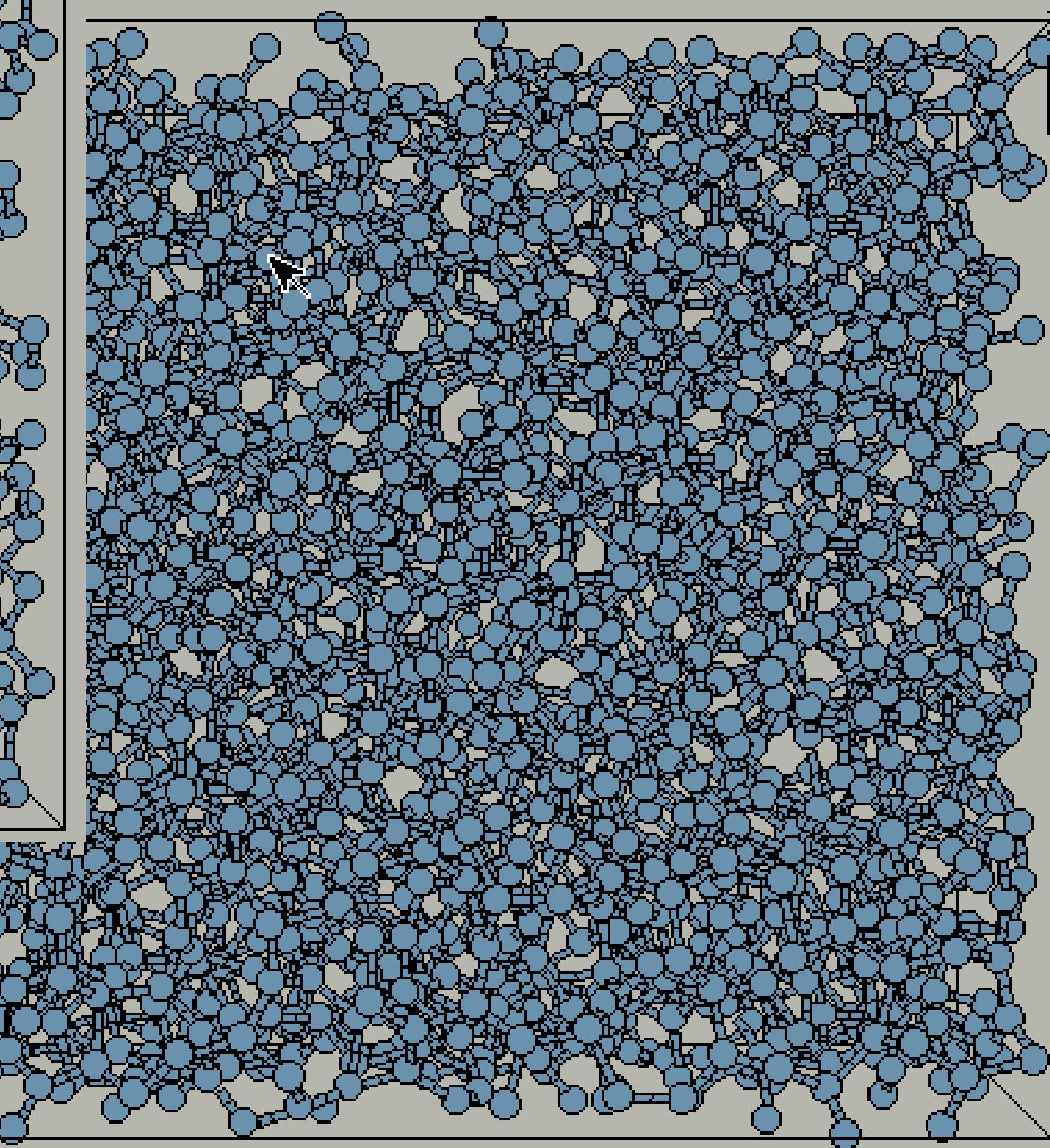
2.0 g/cm³



2.6 g/cm³

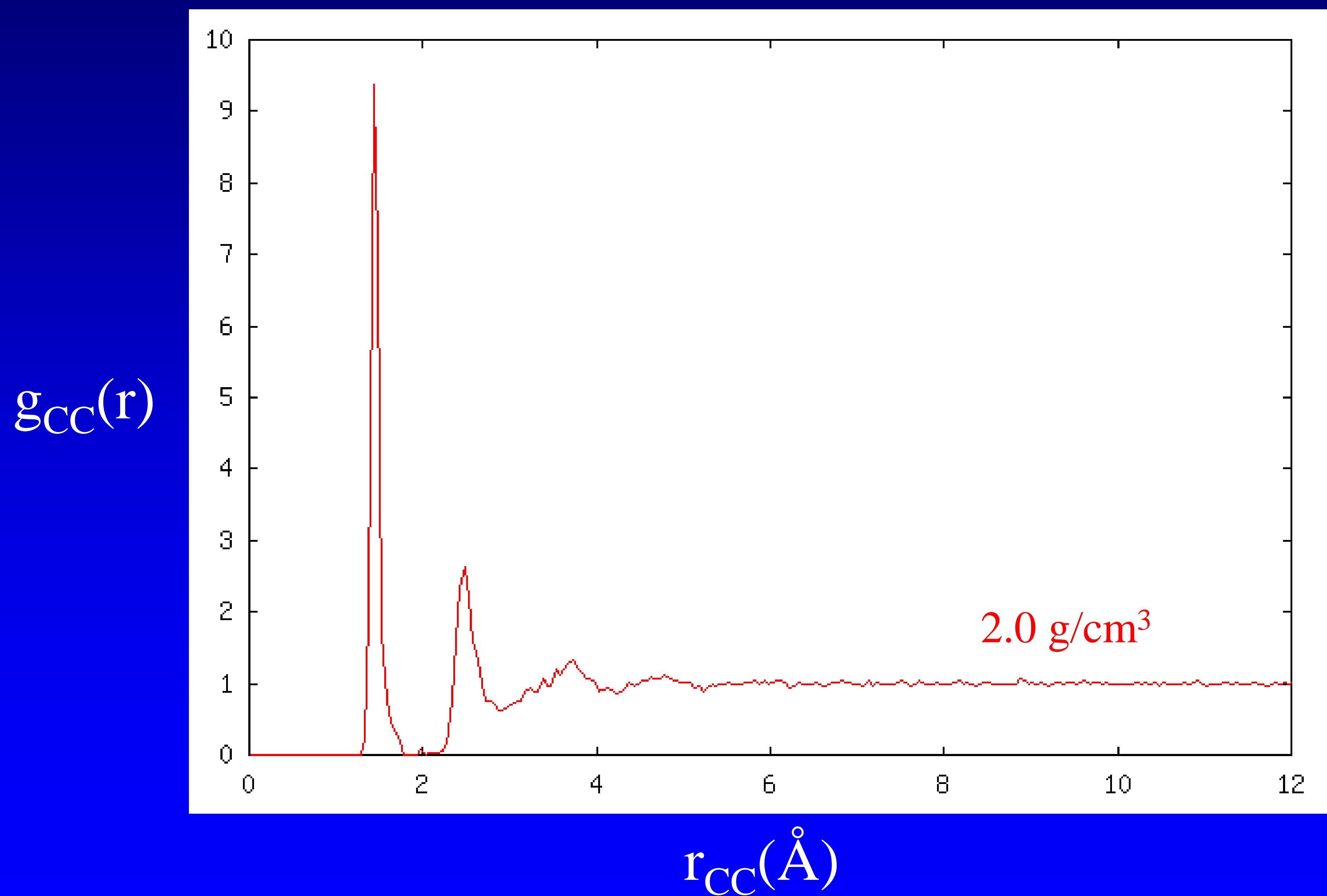


3.0 g/cm³

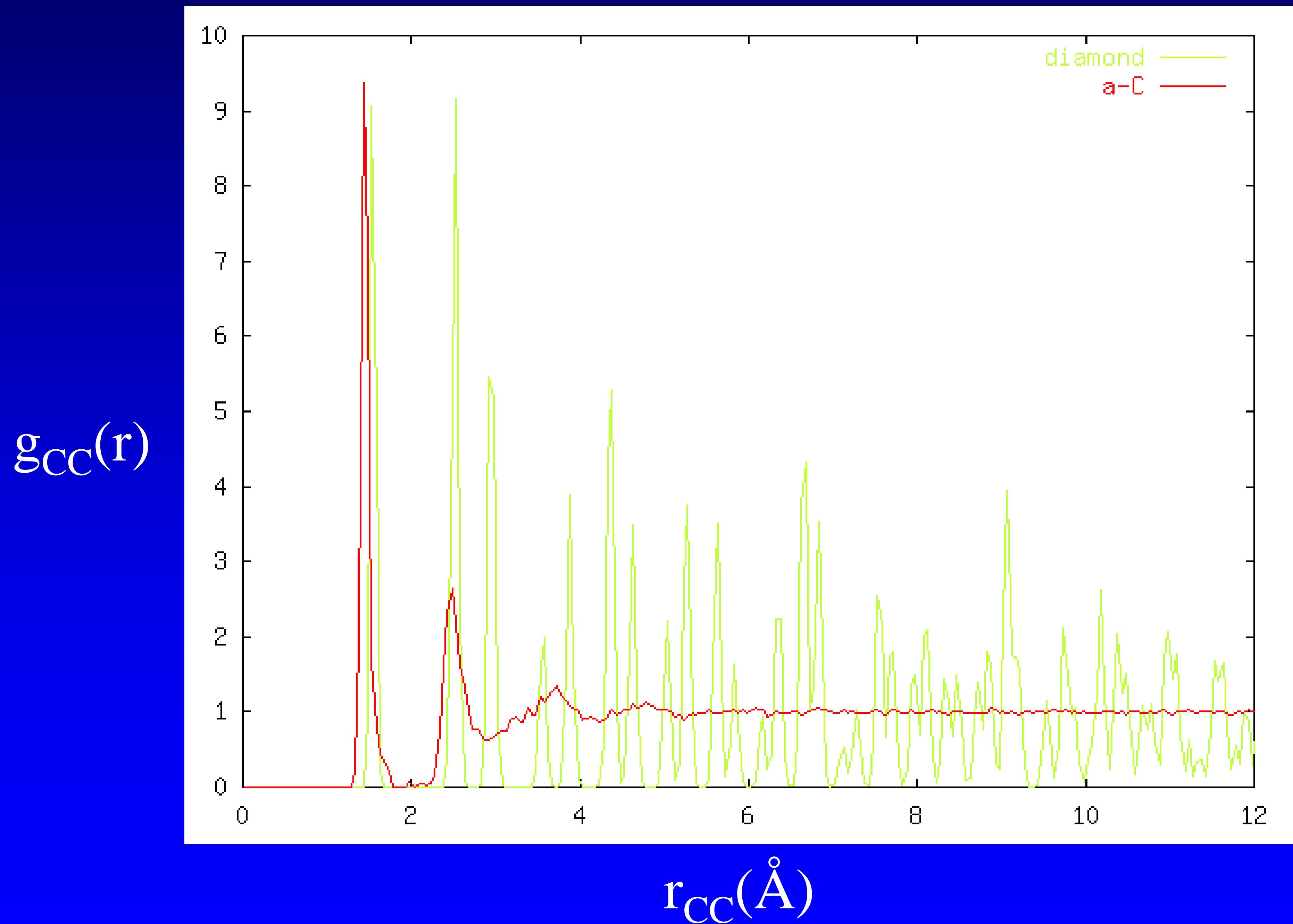


- 50 ps equil at 5000 K
- Quench at 500 K/ps
- Adaptive variable timestep

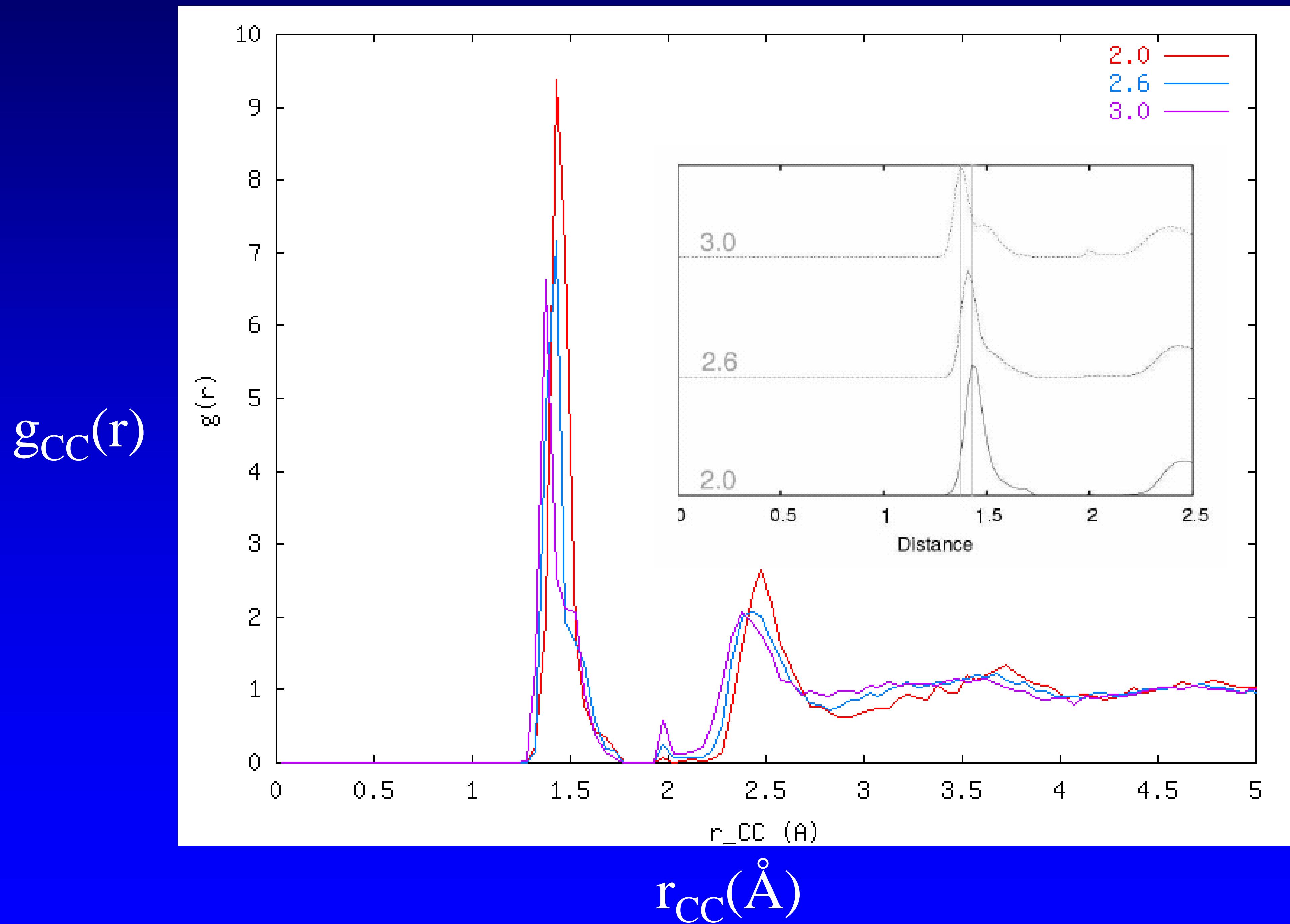
Pair Distribution Function



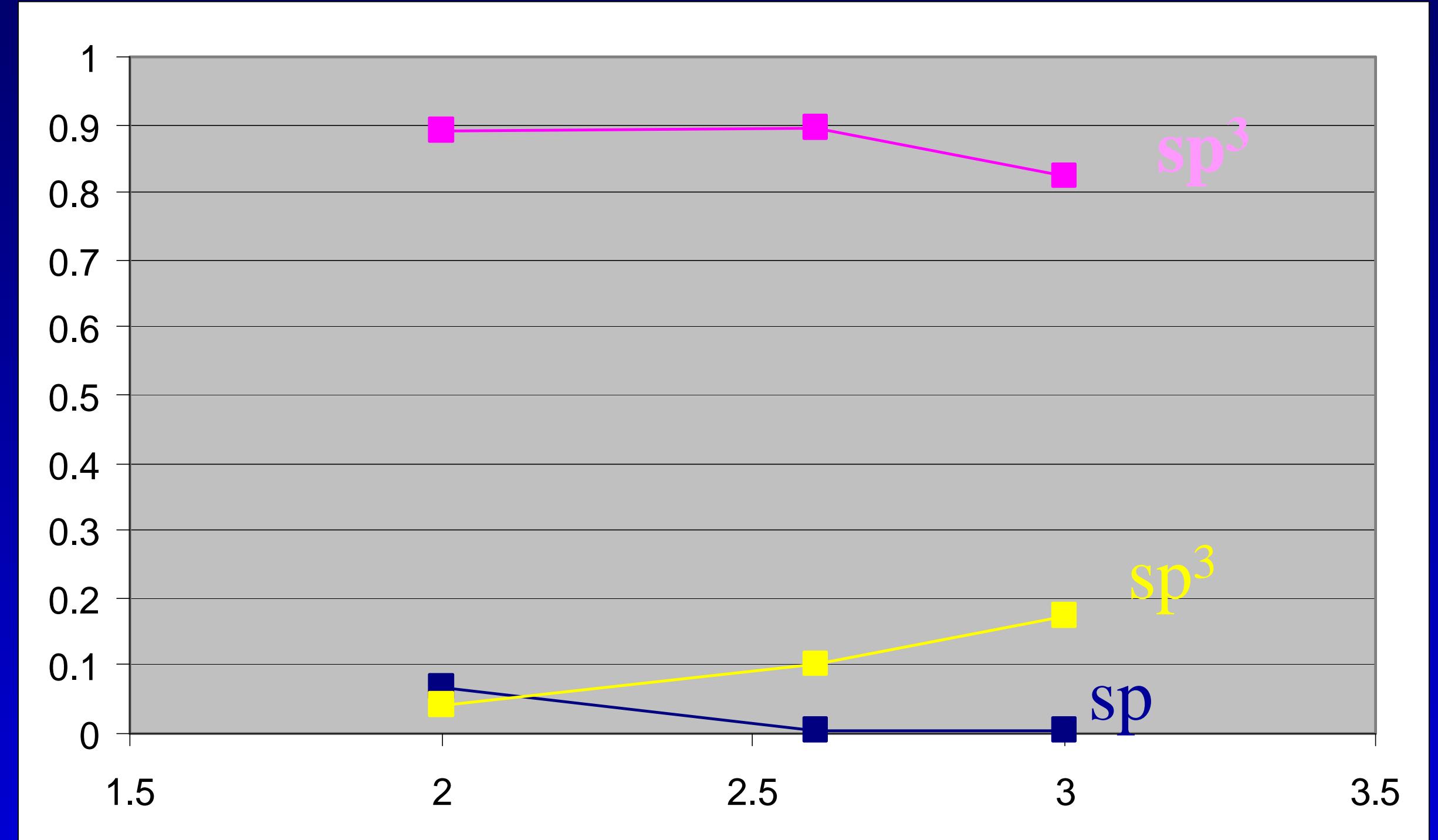
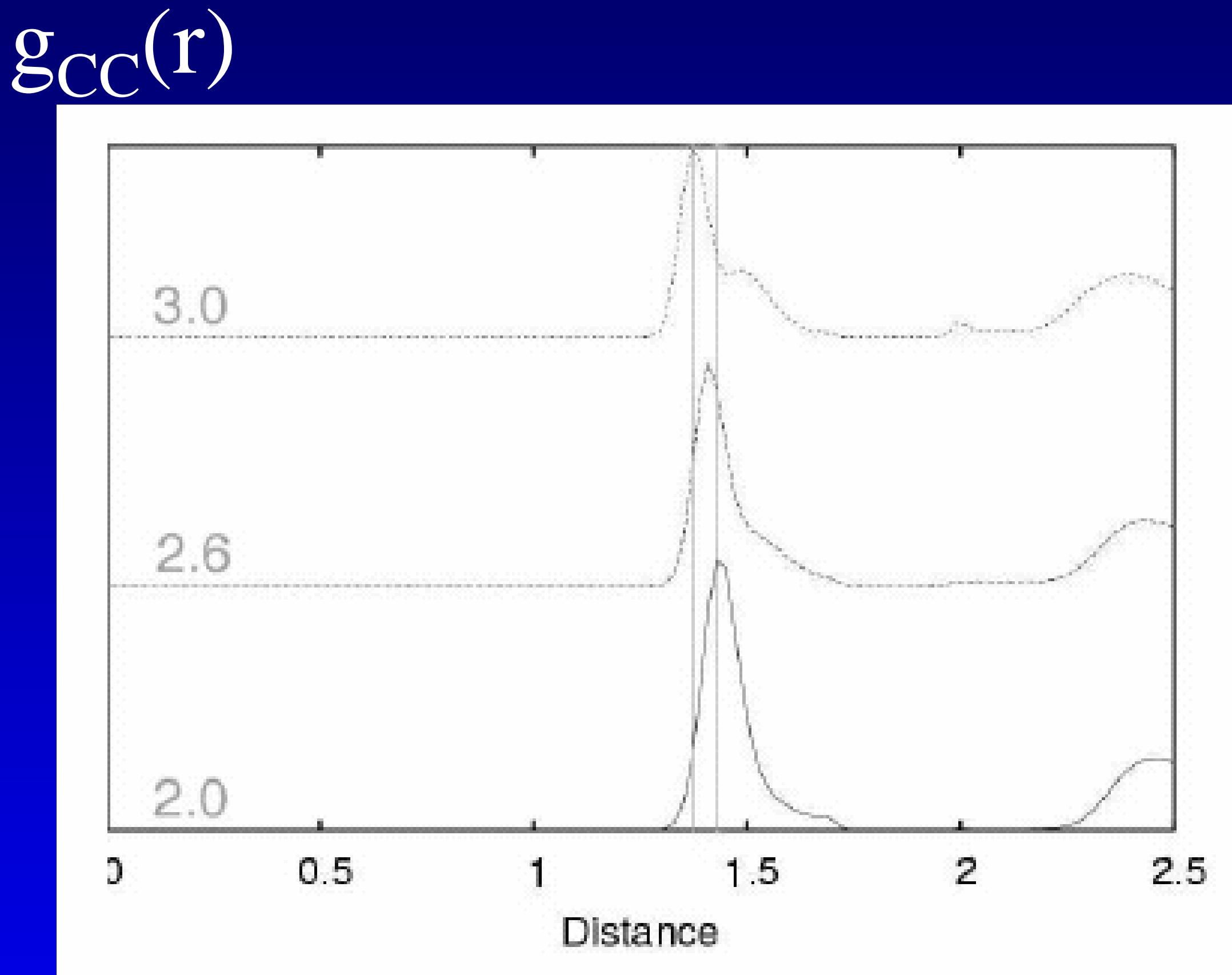
Pair Distribution Function



Pair Distribution Function

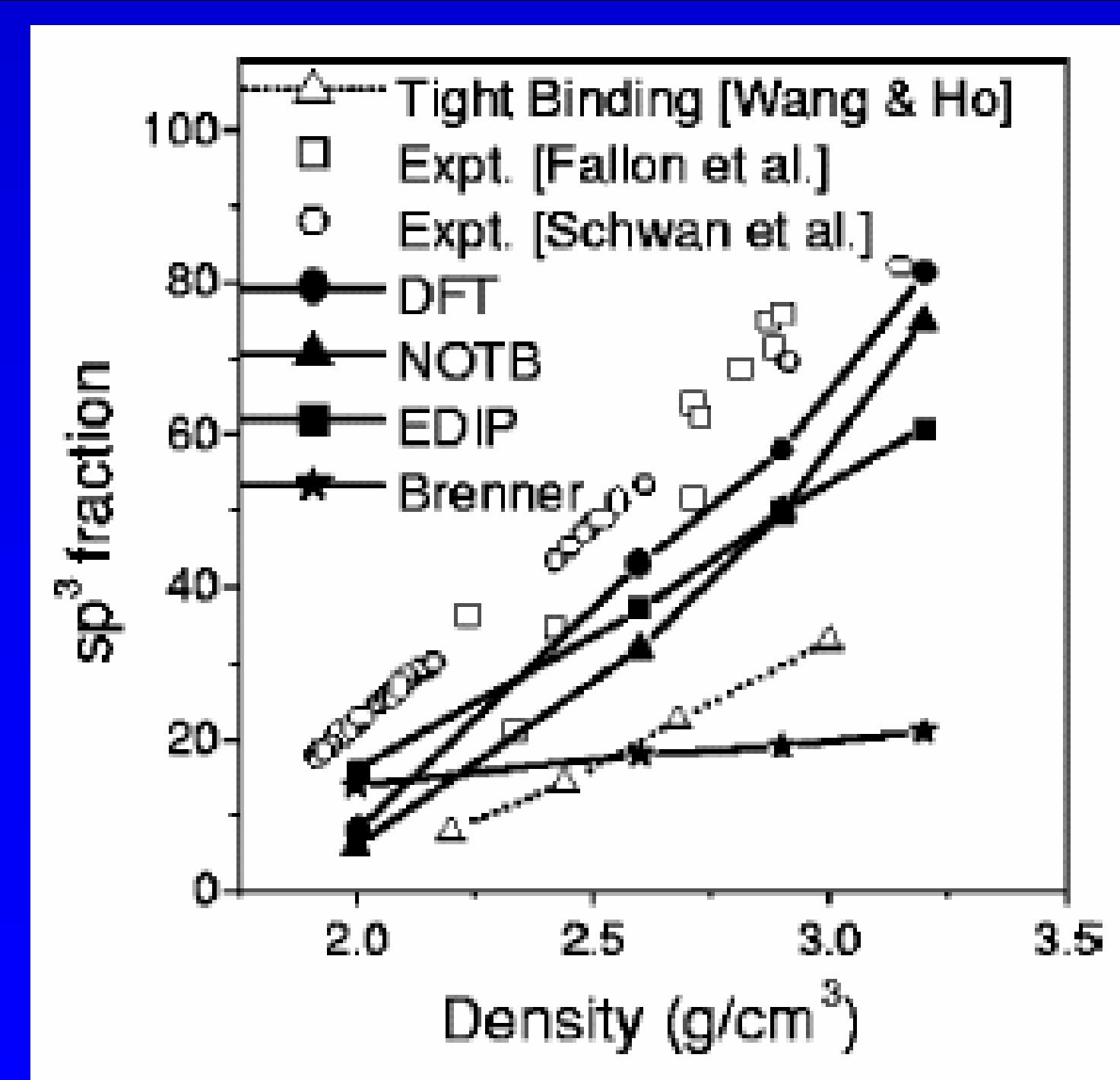


Coordination Number

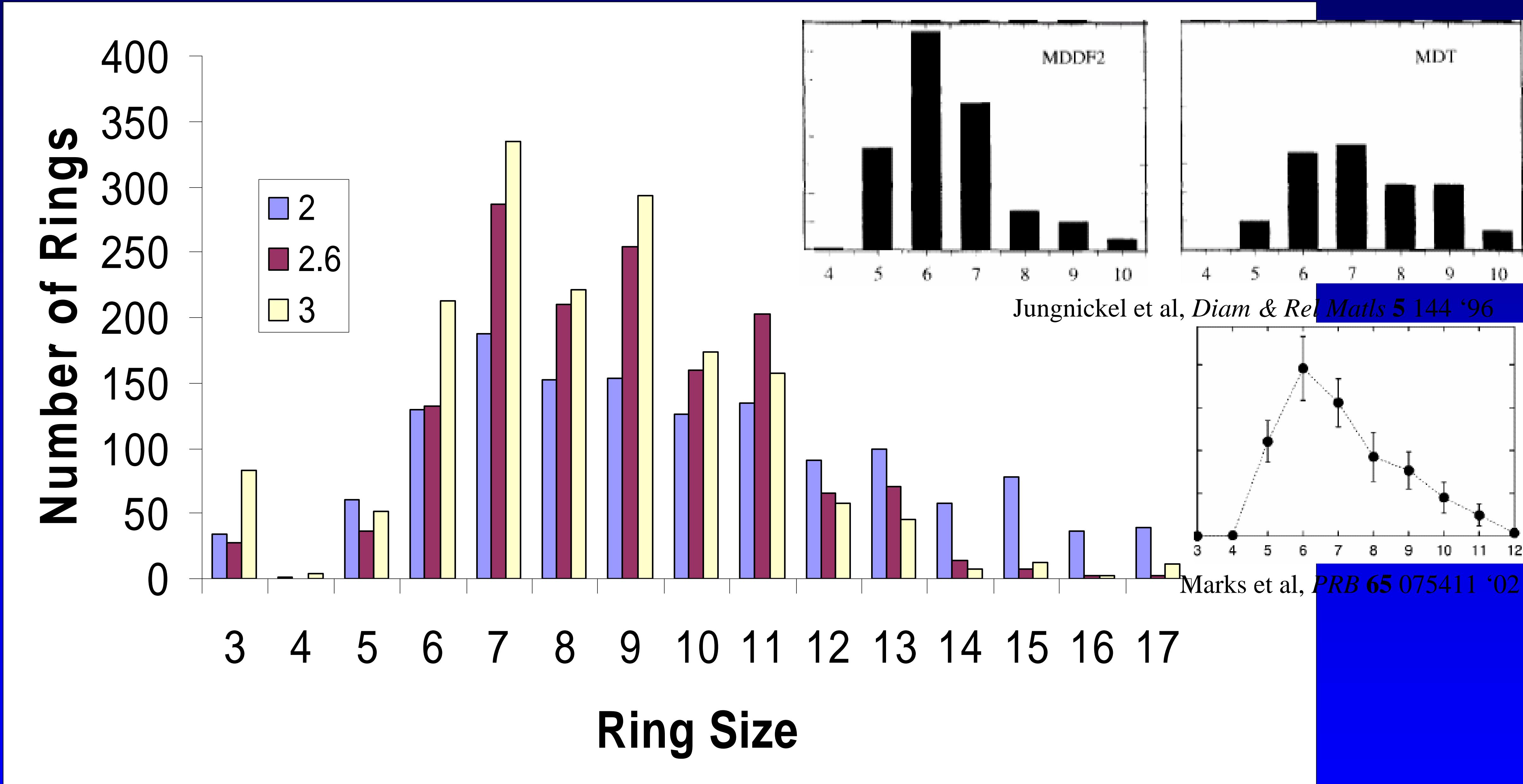


$r_{CC}(\text{\AA})$

REBO and AIREBO
overestimate sp^2
fraction



Ring Size Distribution

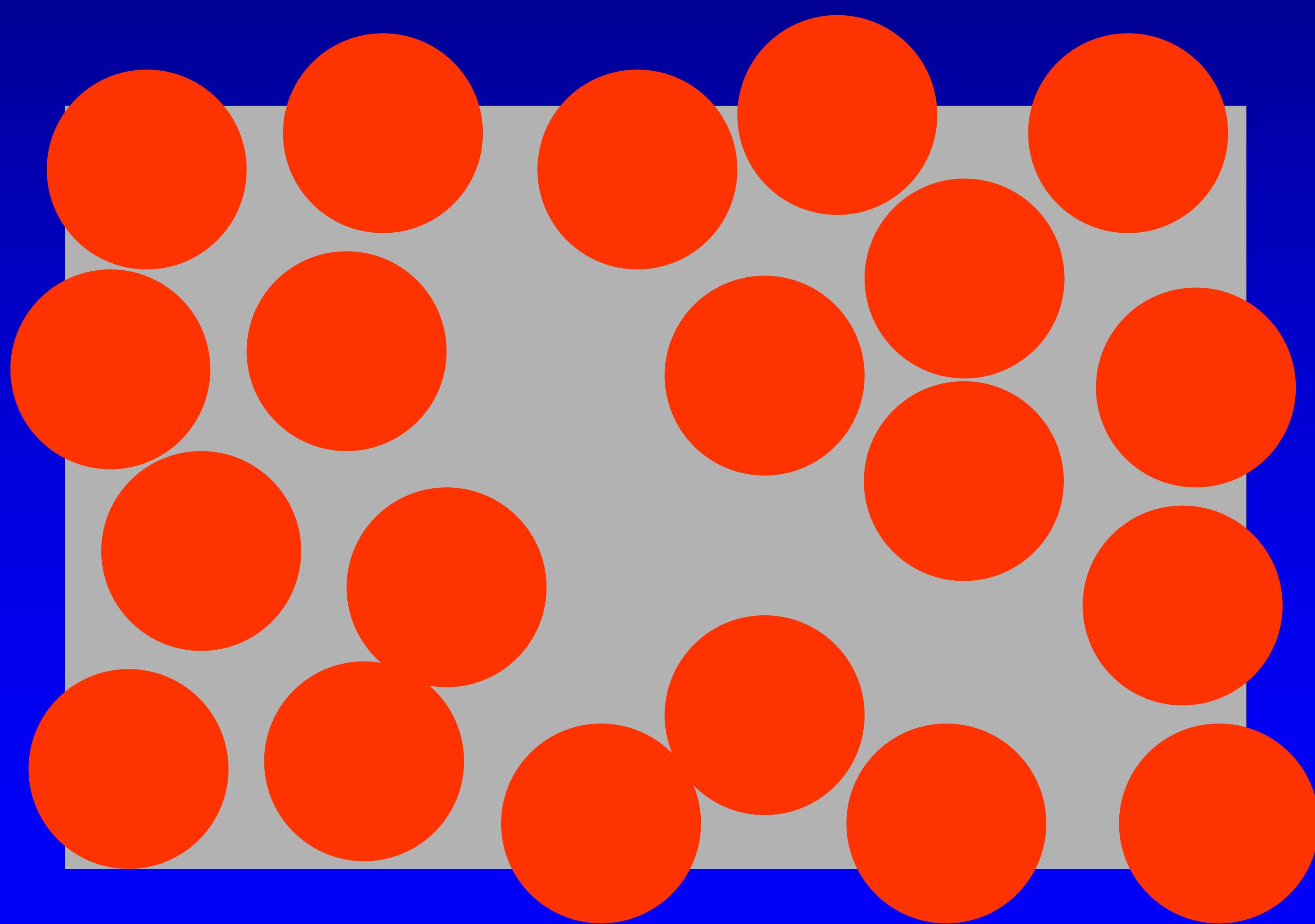


- Ambiguous definition
- Franzblau SP rings

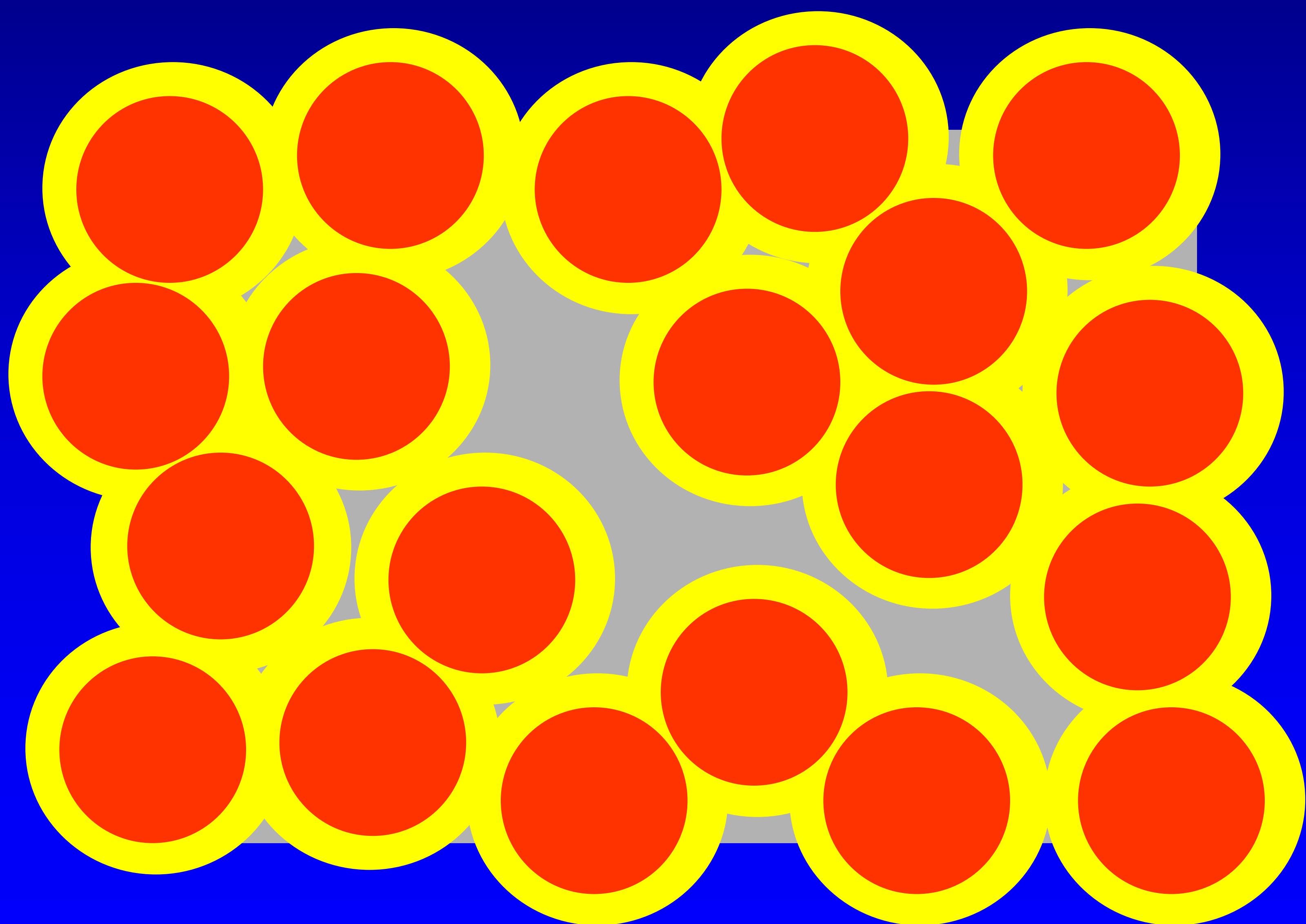
DS Franzblau *PRB* 44 4925 '91

- Even/odd alternation
- Cyclopropyl rings underpenalized

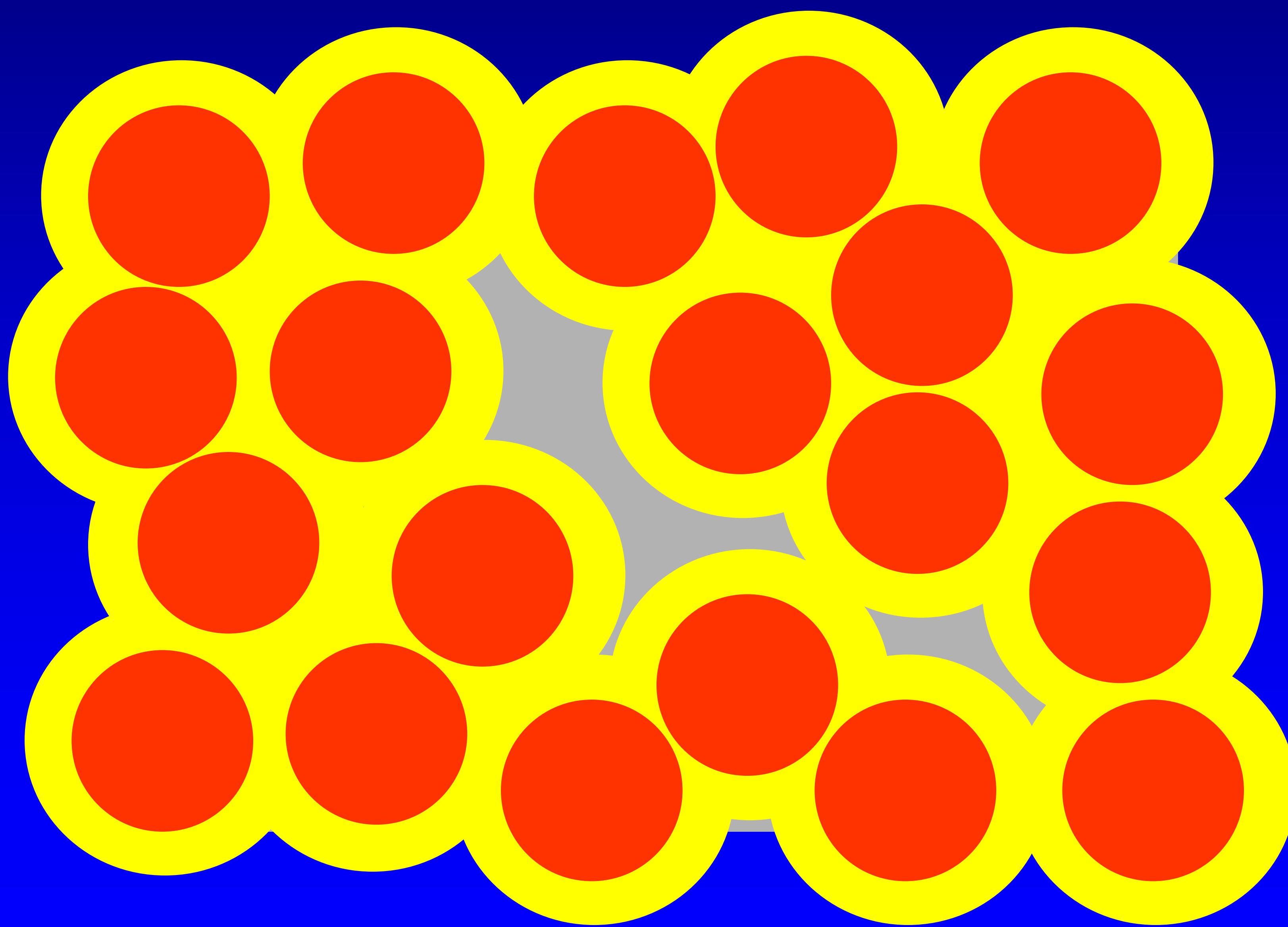
Void Sizes



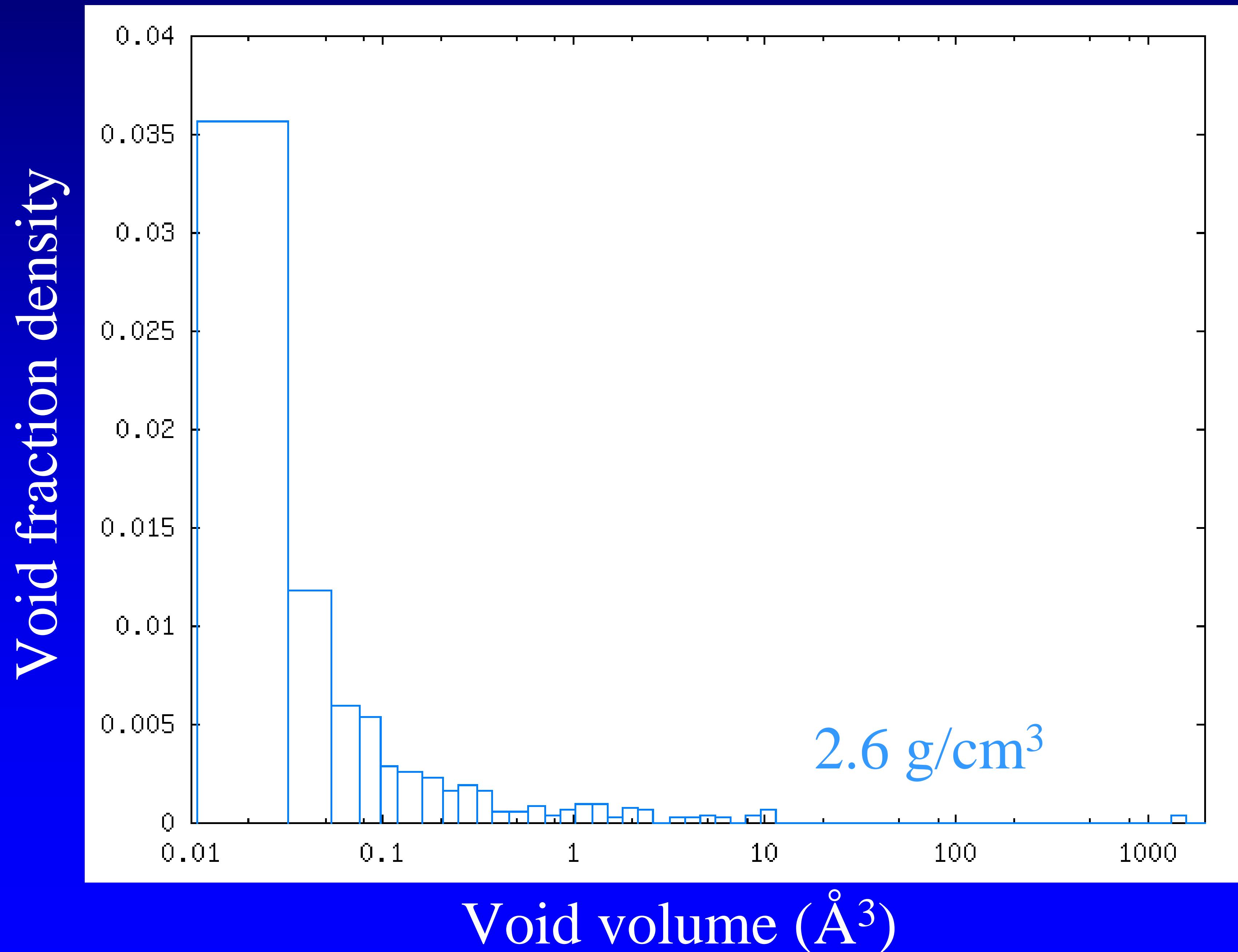
Void Sizes



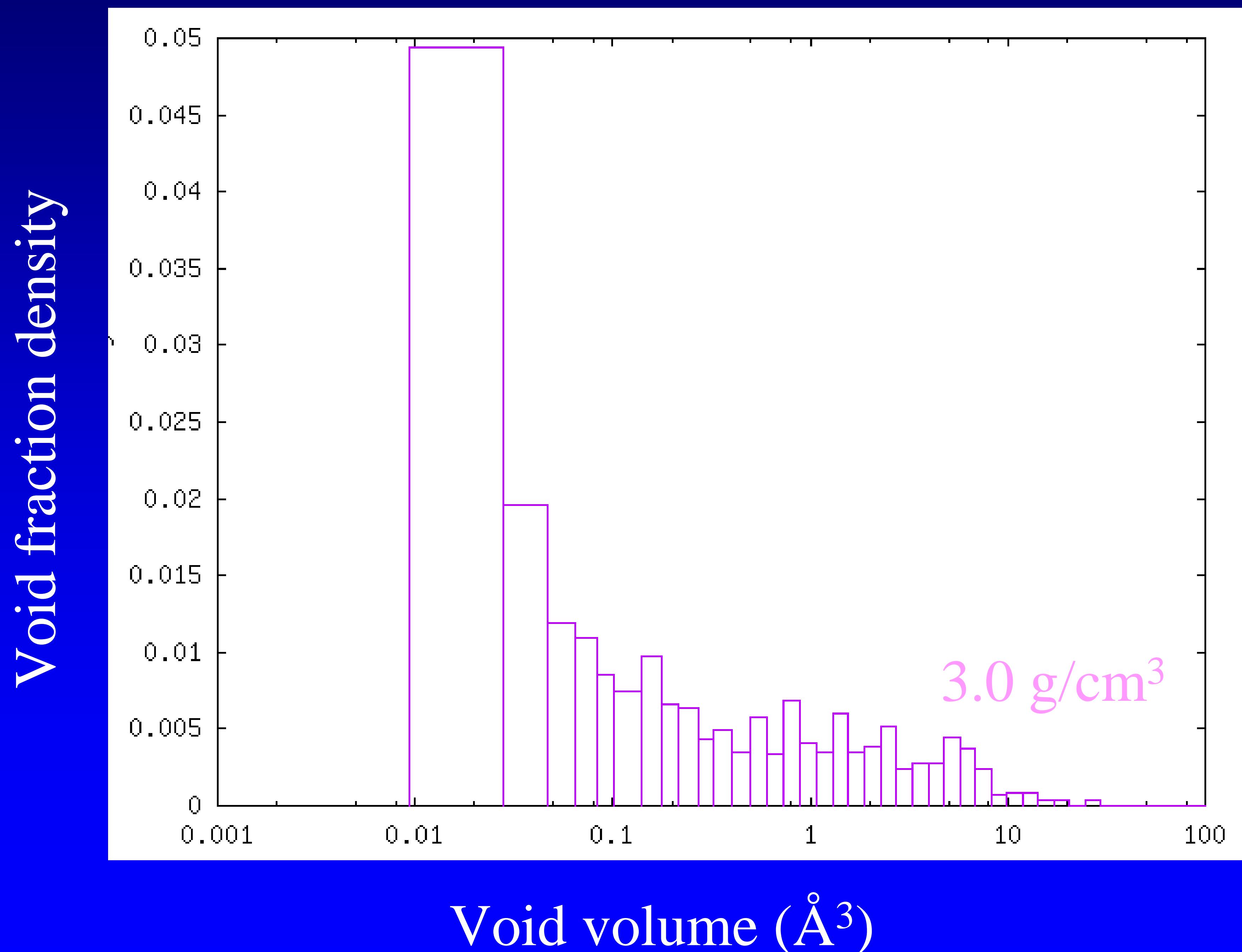
Void Sizes



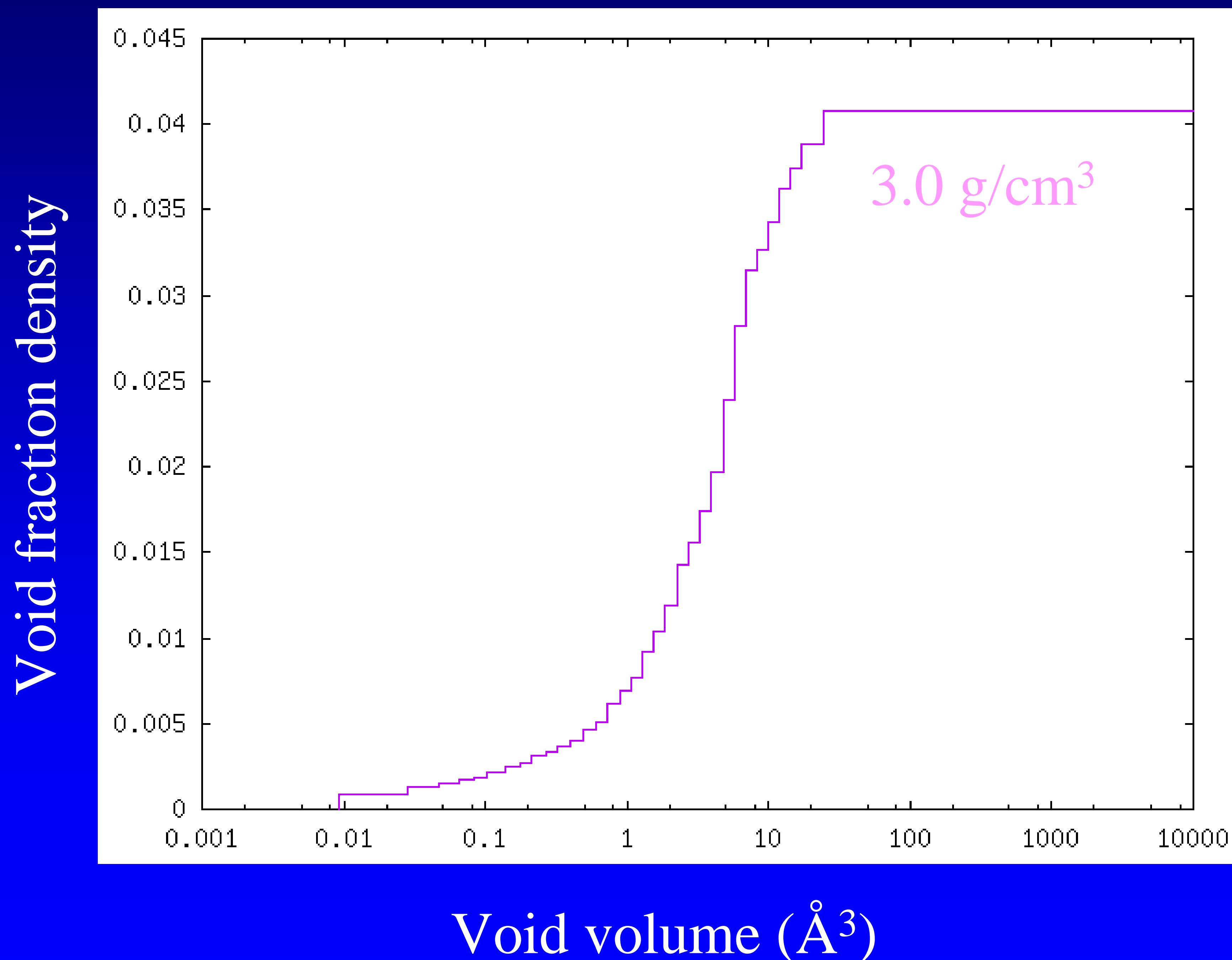
Void Volume Distribution



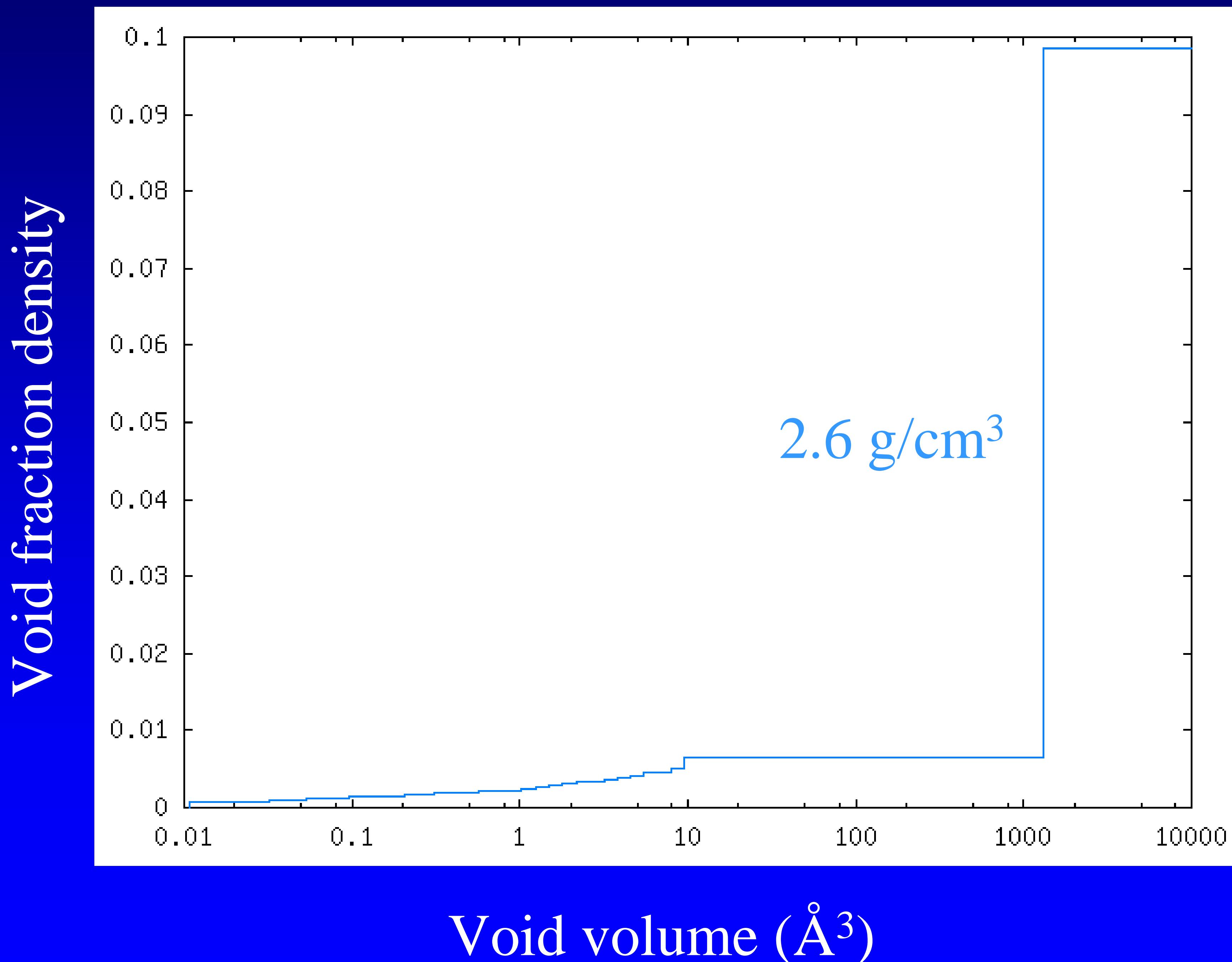
Void Volume Distribution



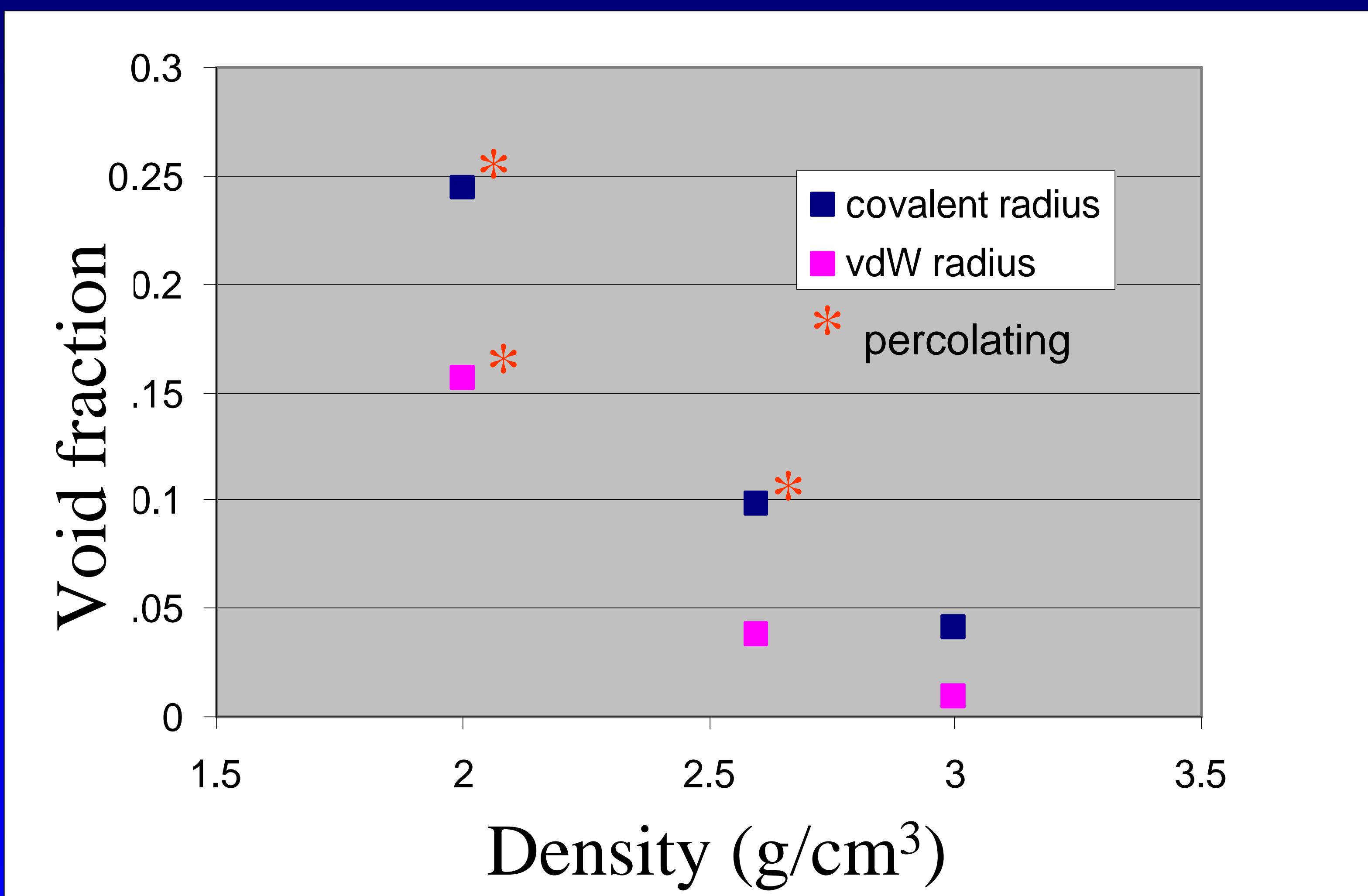
Void Volume Distribution



Void Volume Distribution

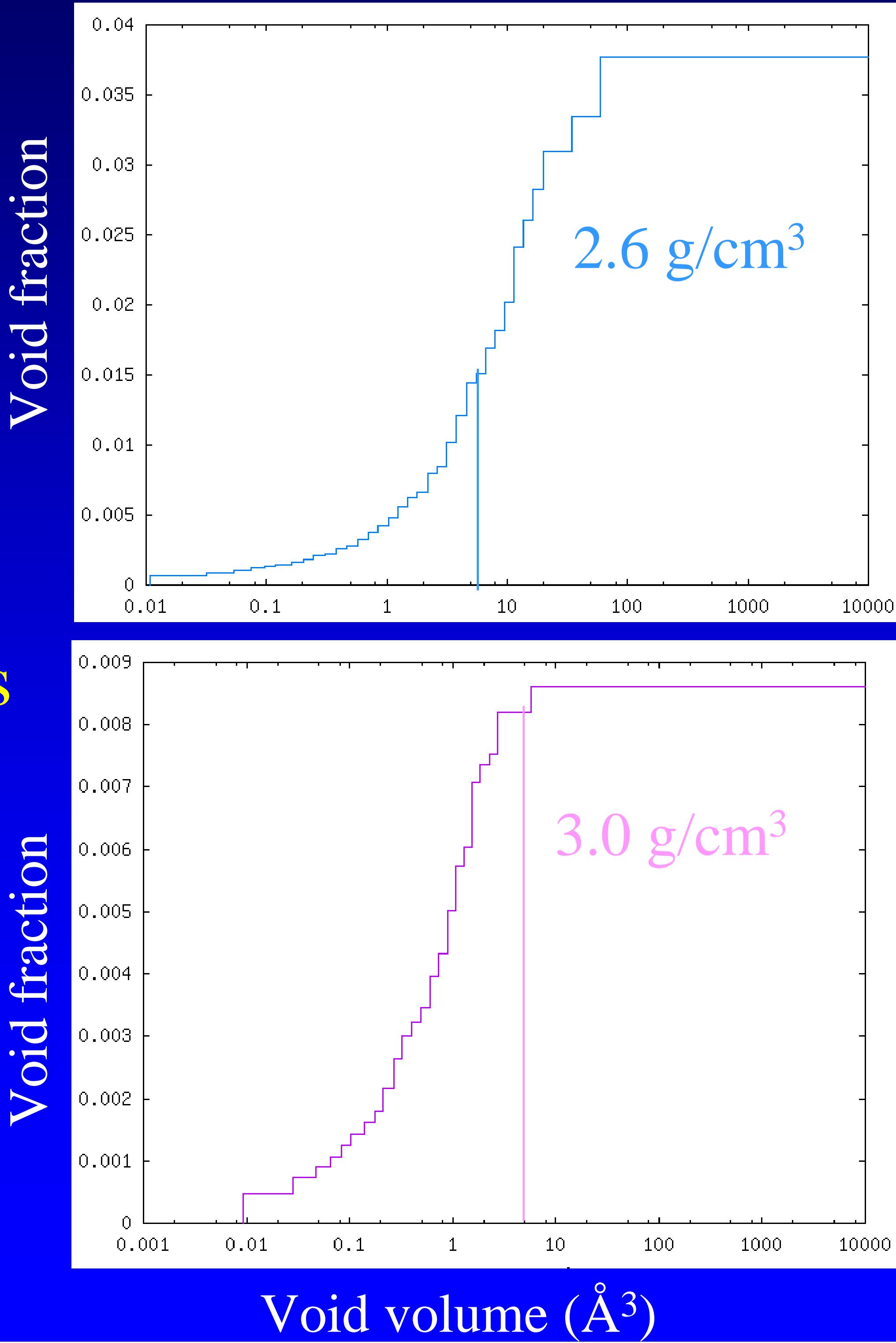


Void Volume Distribution

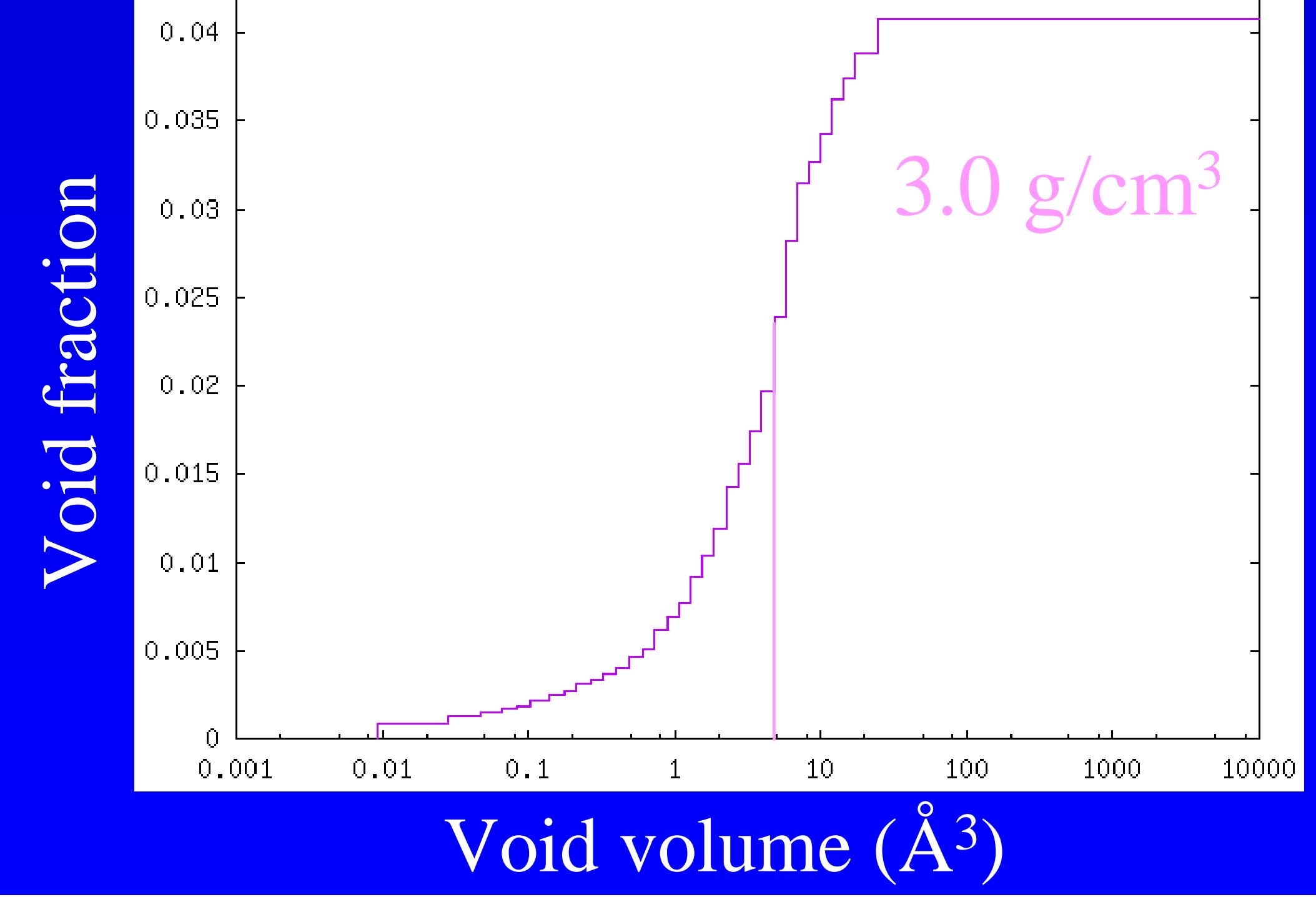


Void Volume Distribution

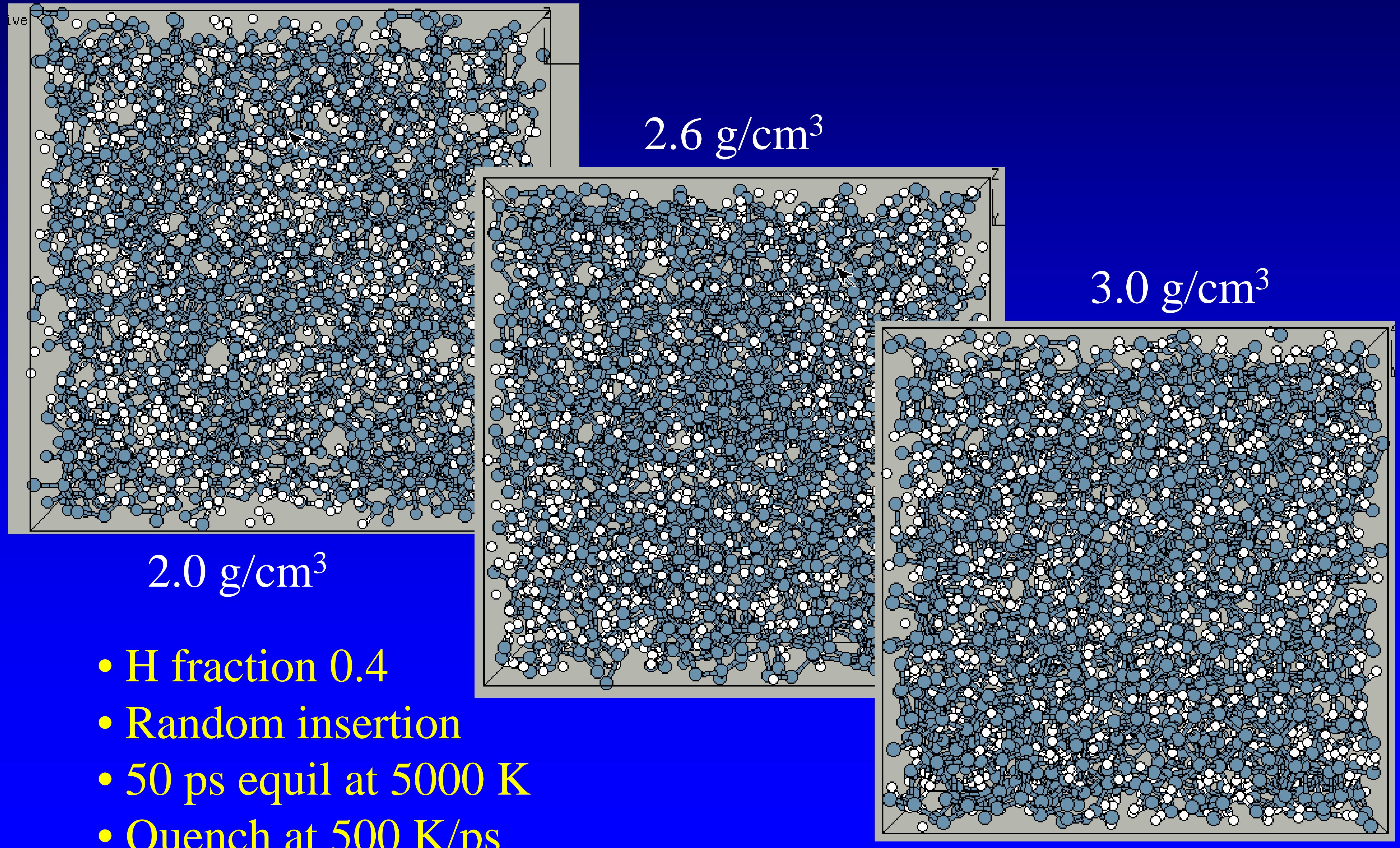
vdW
voids



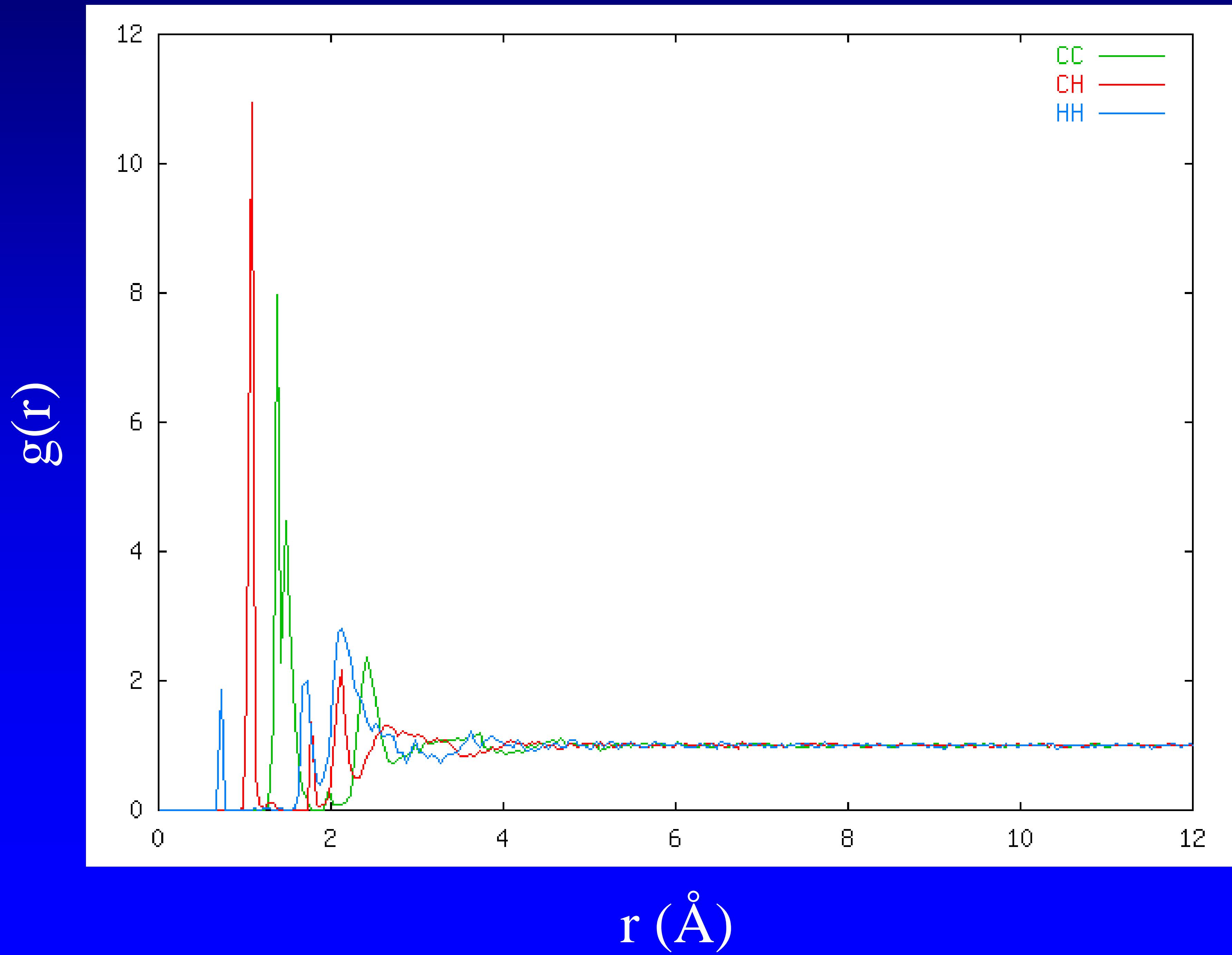
covalent voids



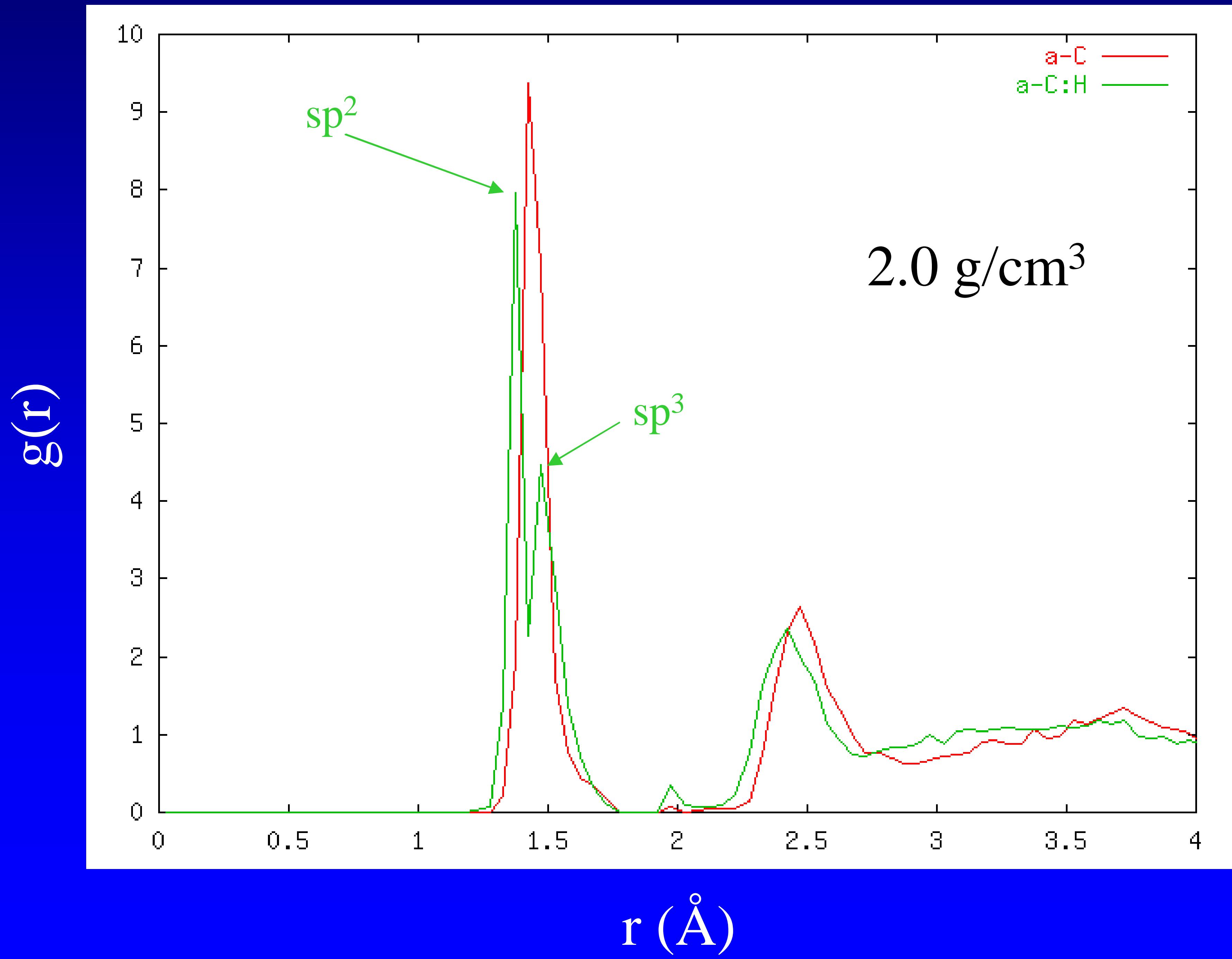
a-C:T



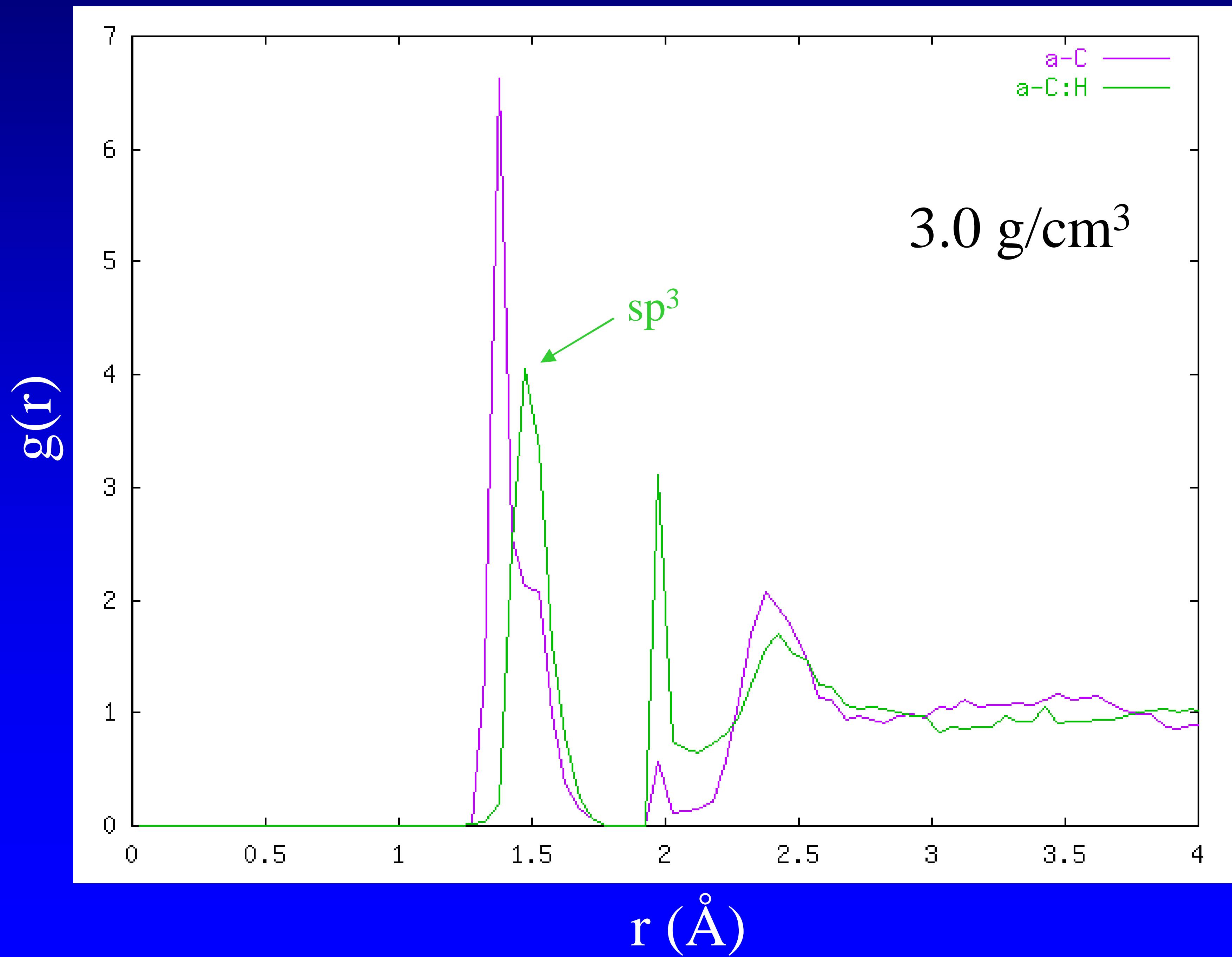
a-C:T Structure



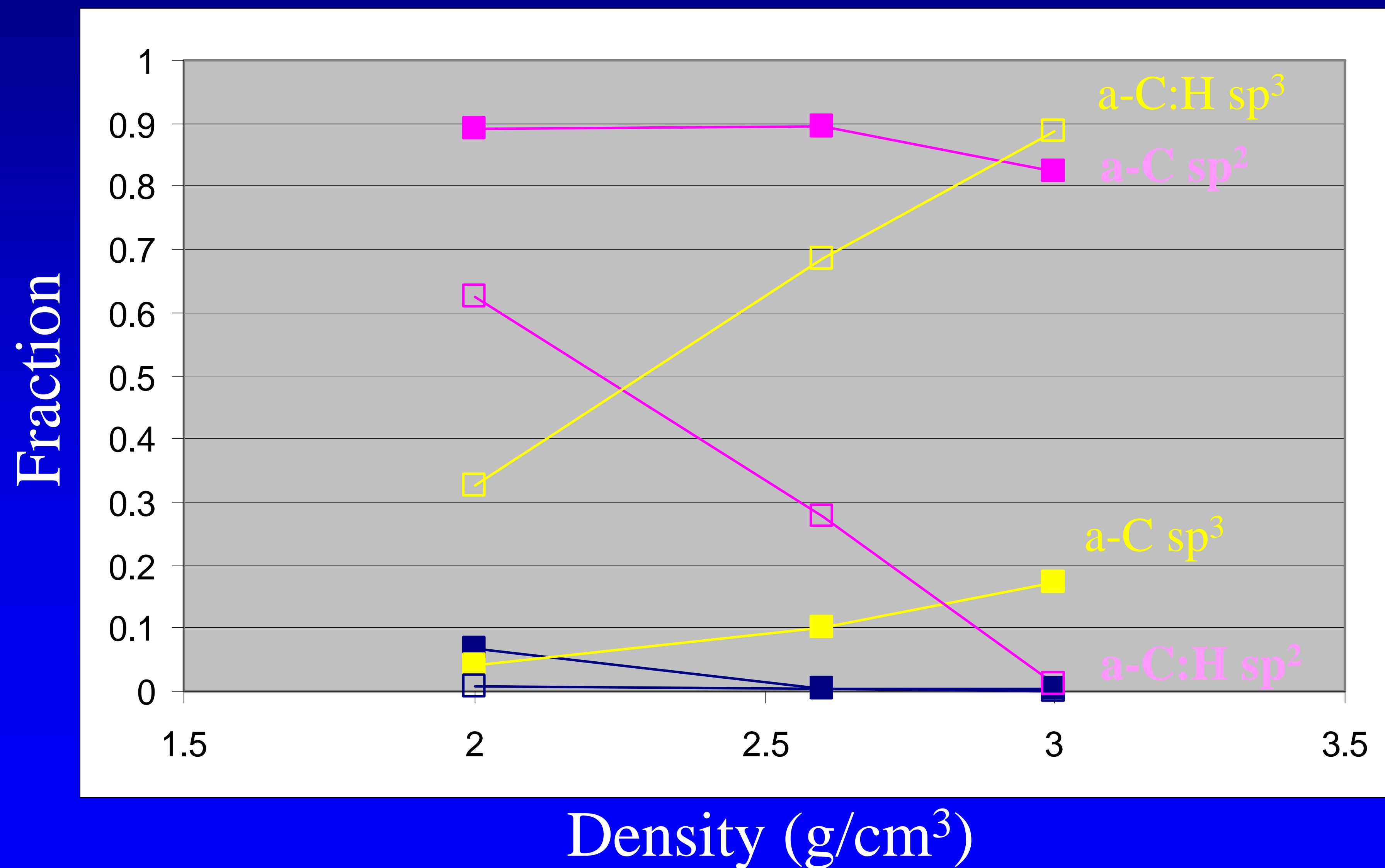
a-C:T Structure



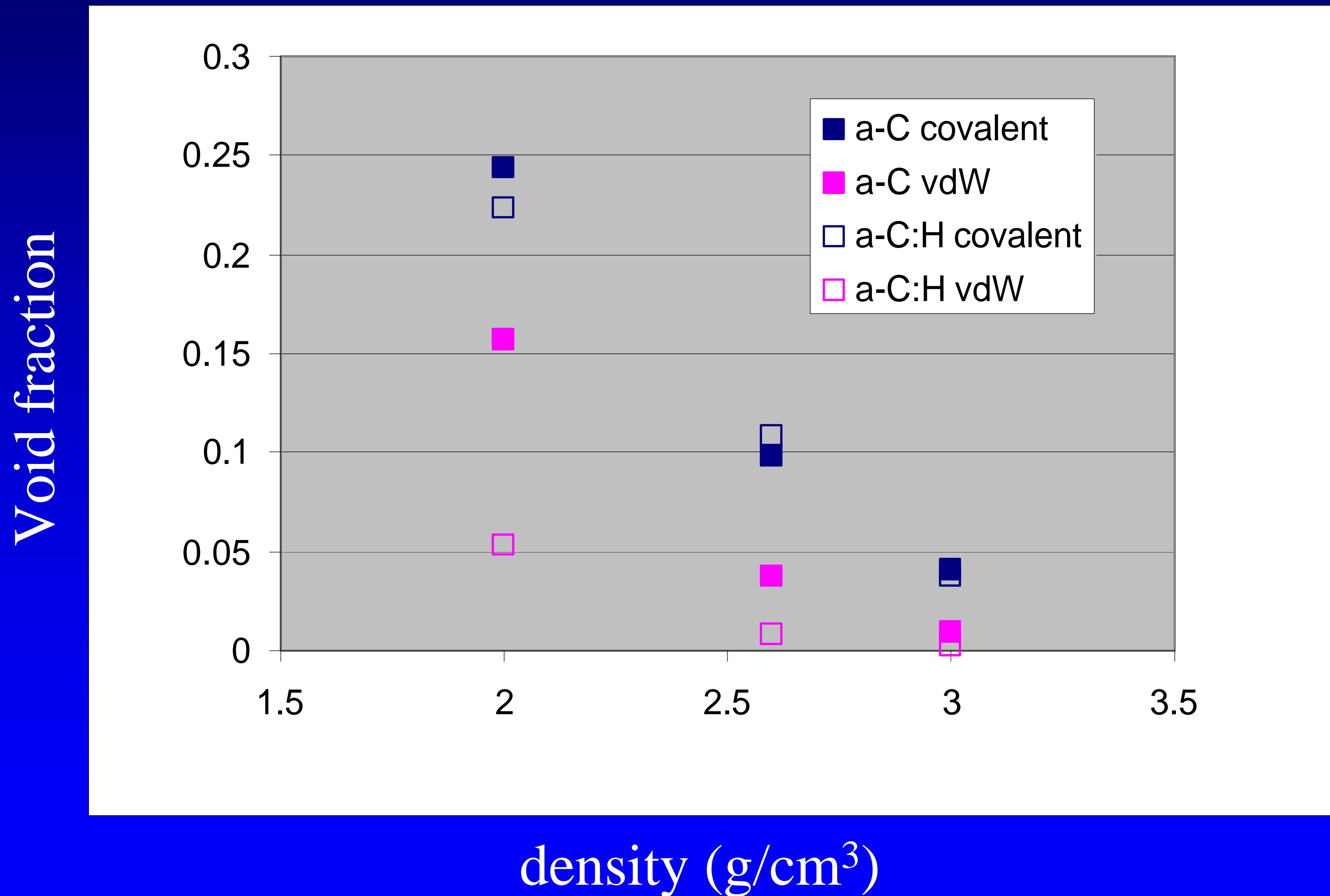
a-C:T Structure



a-C:T Coordination Number

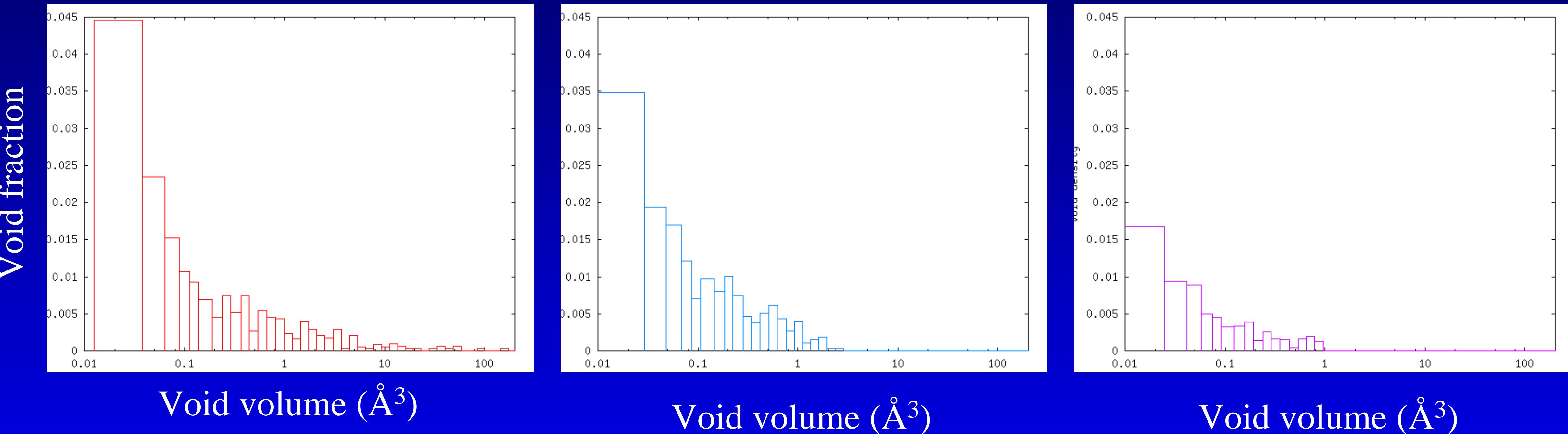


a-C: 3 H Void Volumes

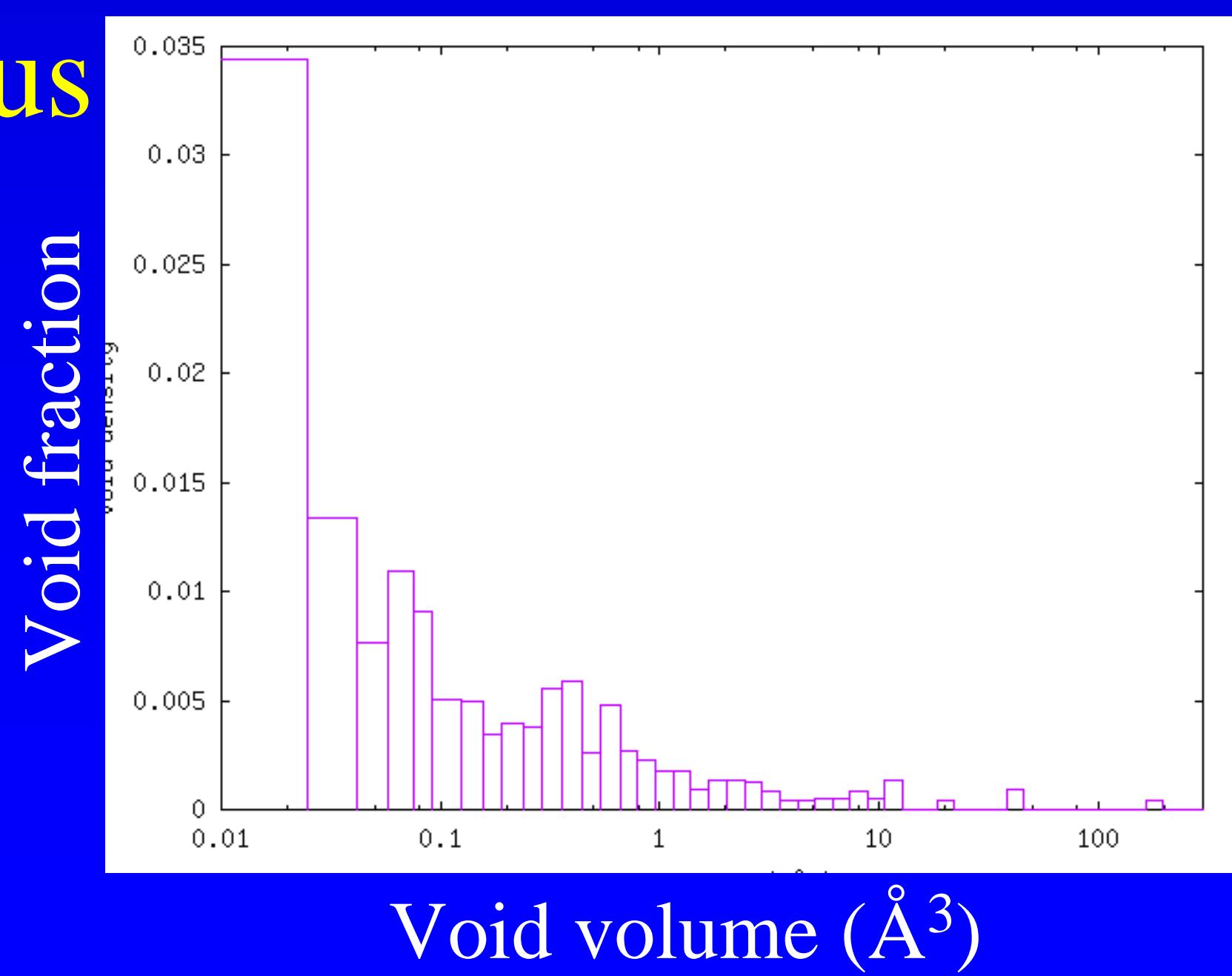


a-C:T Void Volume Distribution

vdW void radius



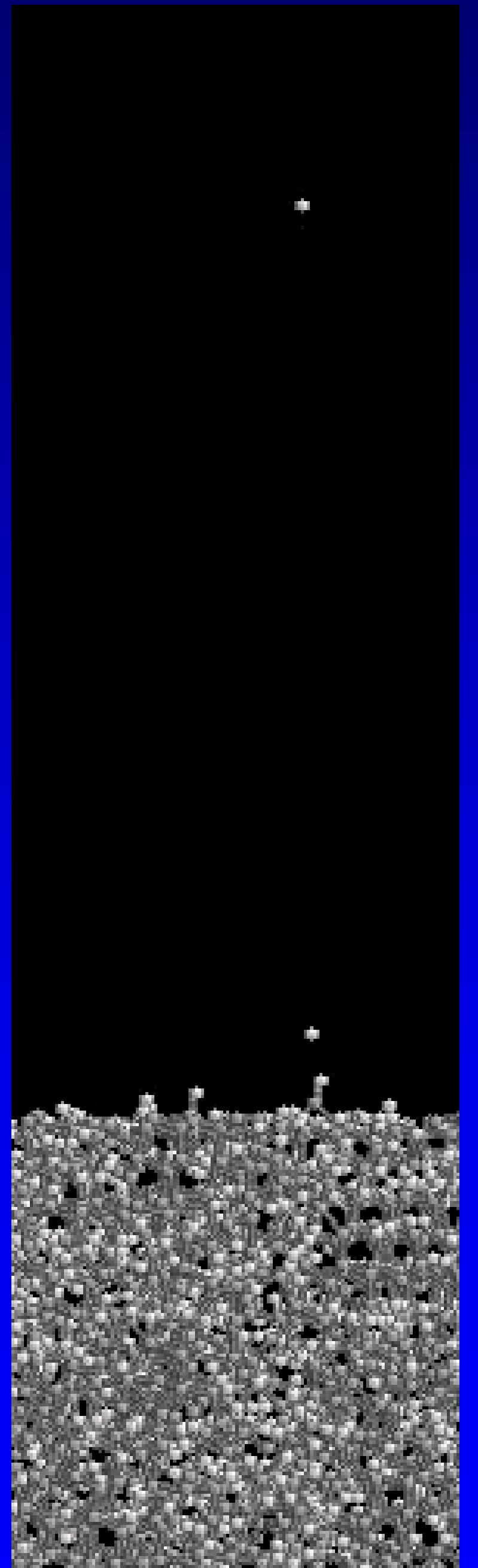
covalent void radius



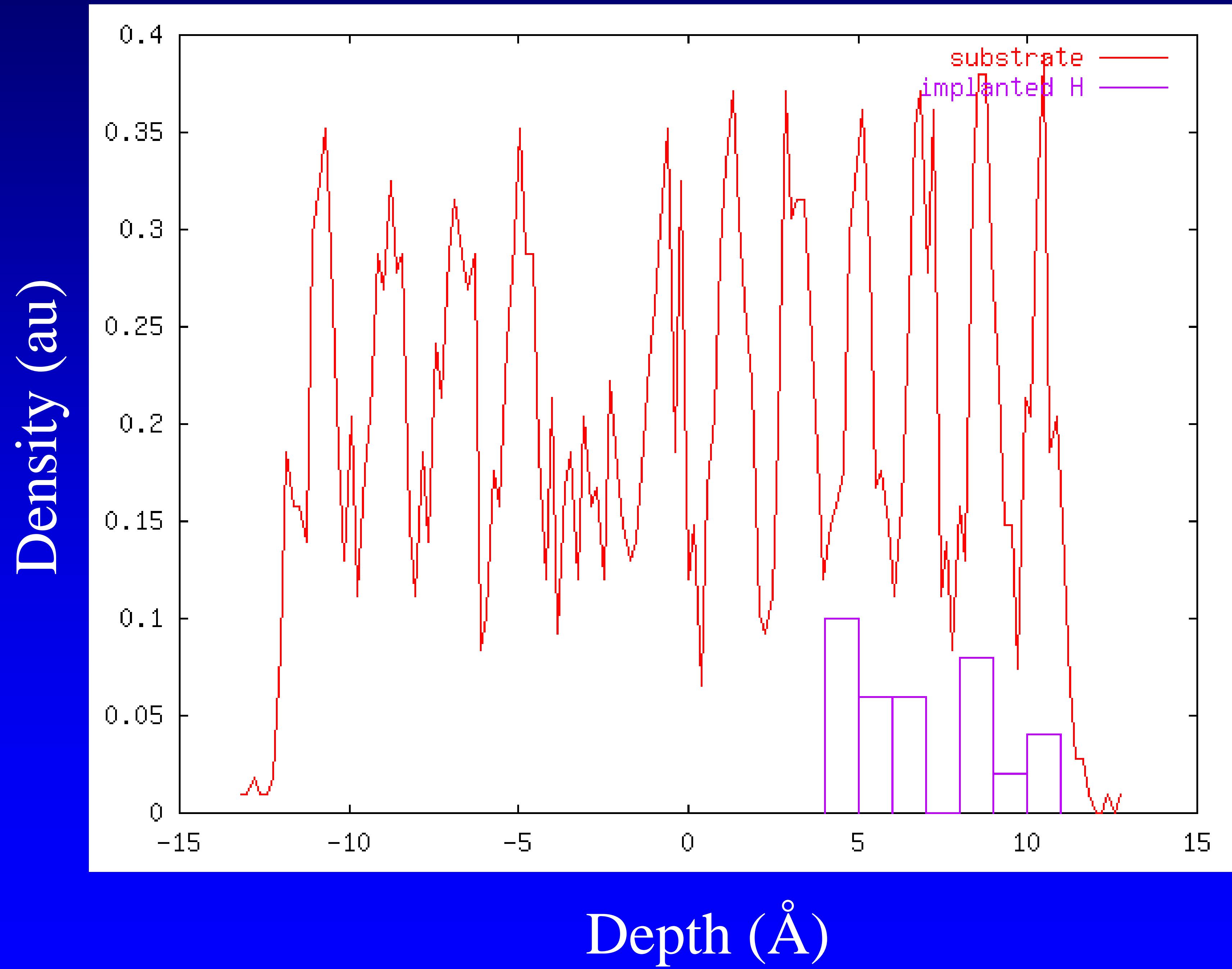
Sputtering of a-C:T



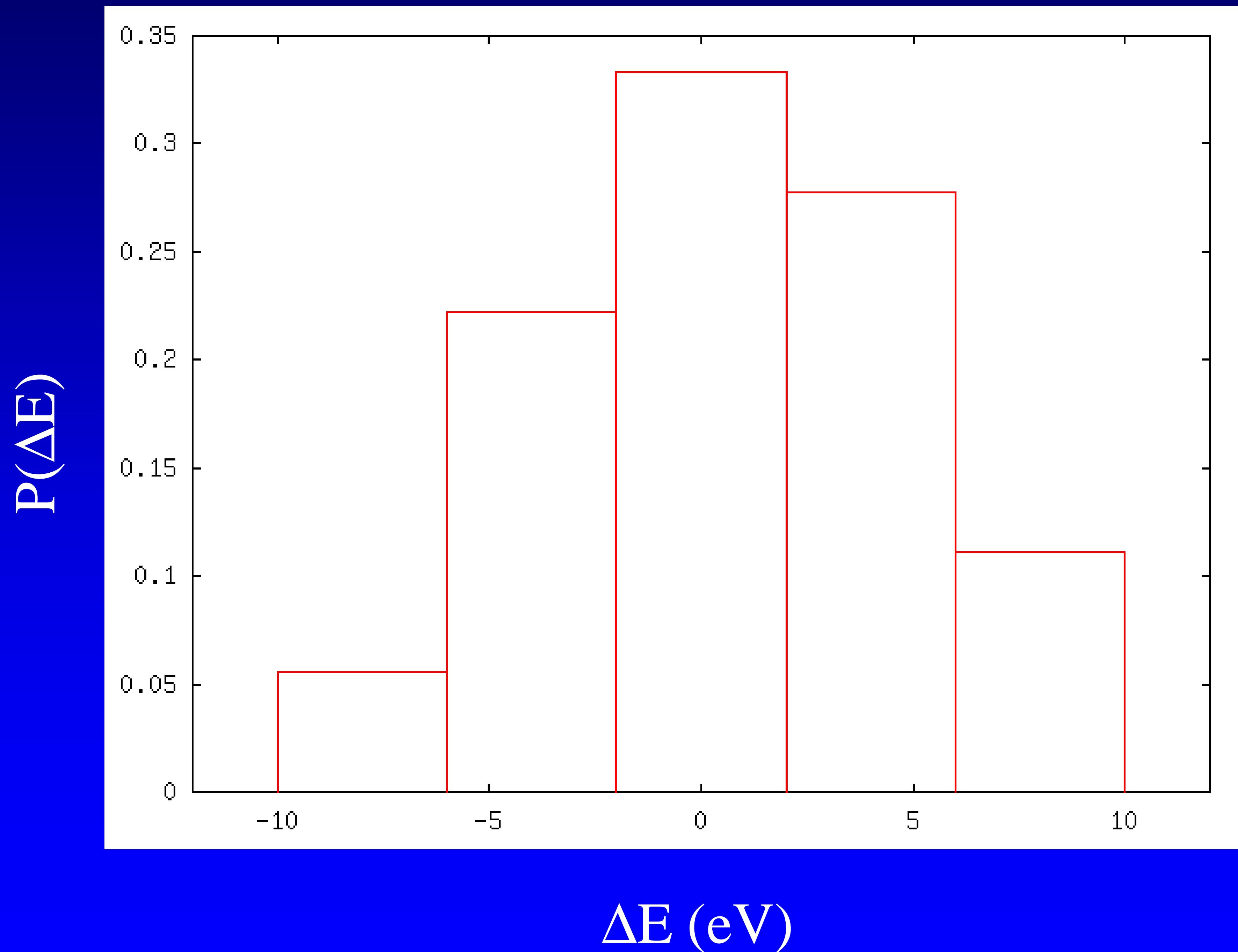
- T ? a-C:T
- 88 eV impacts
- normal incidence
- 3 ps between impacts



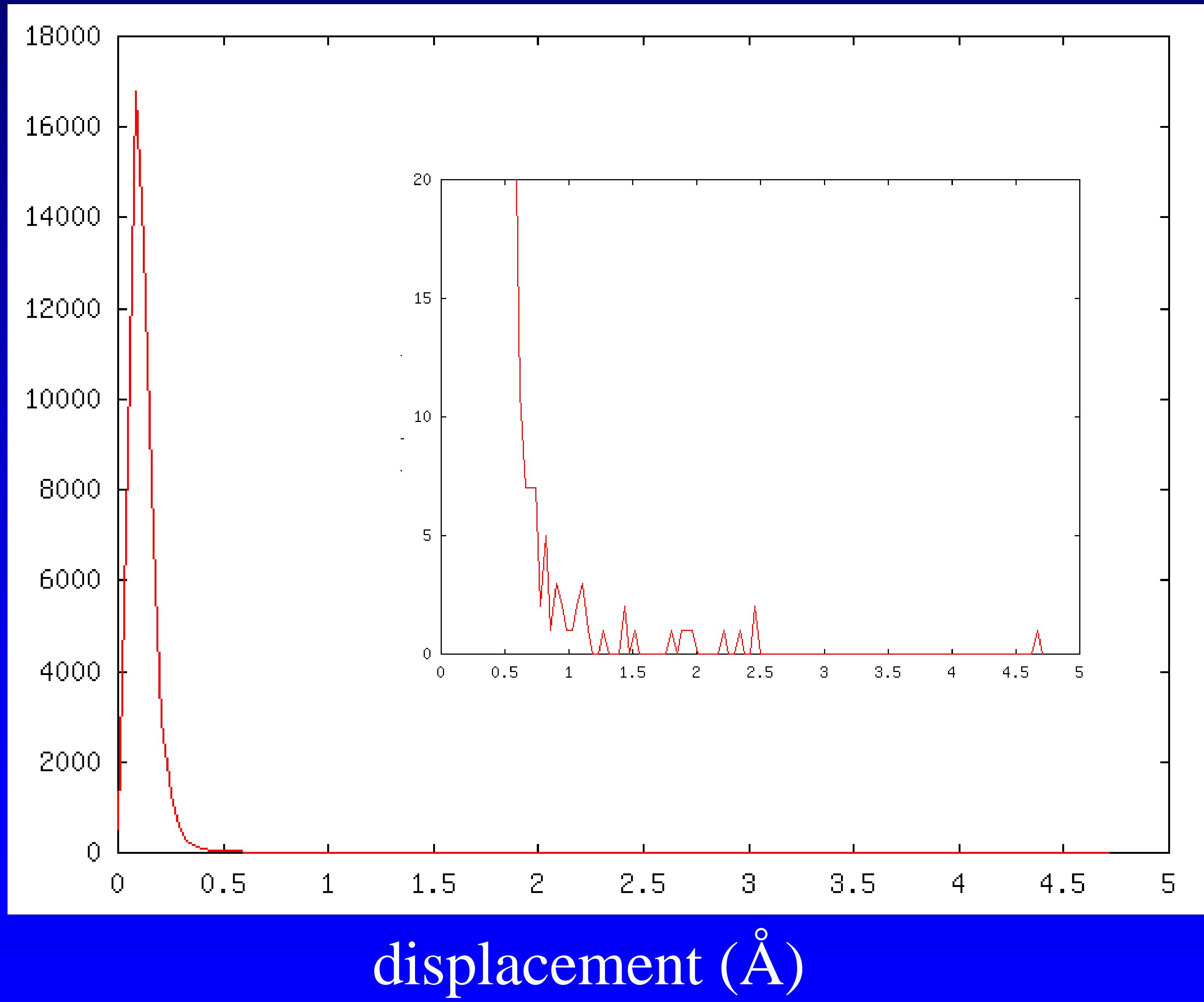
Implantation Depth



Energy Dissipation



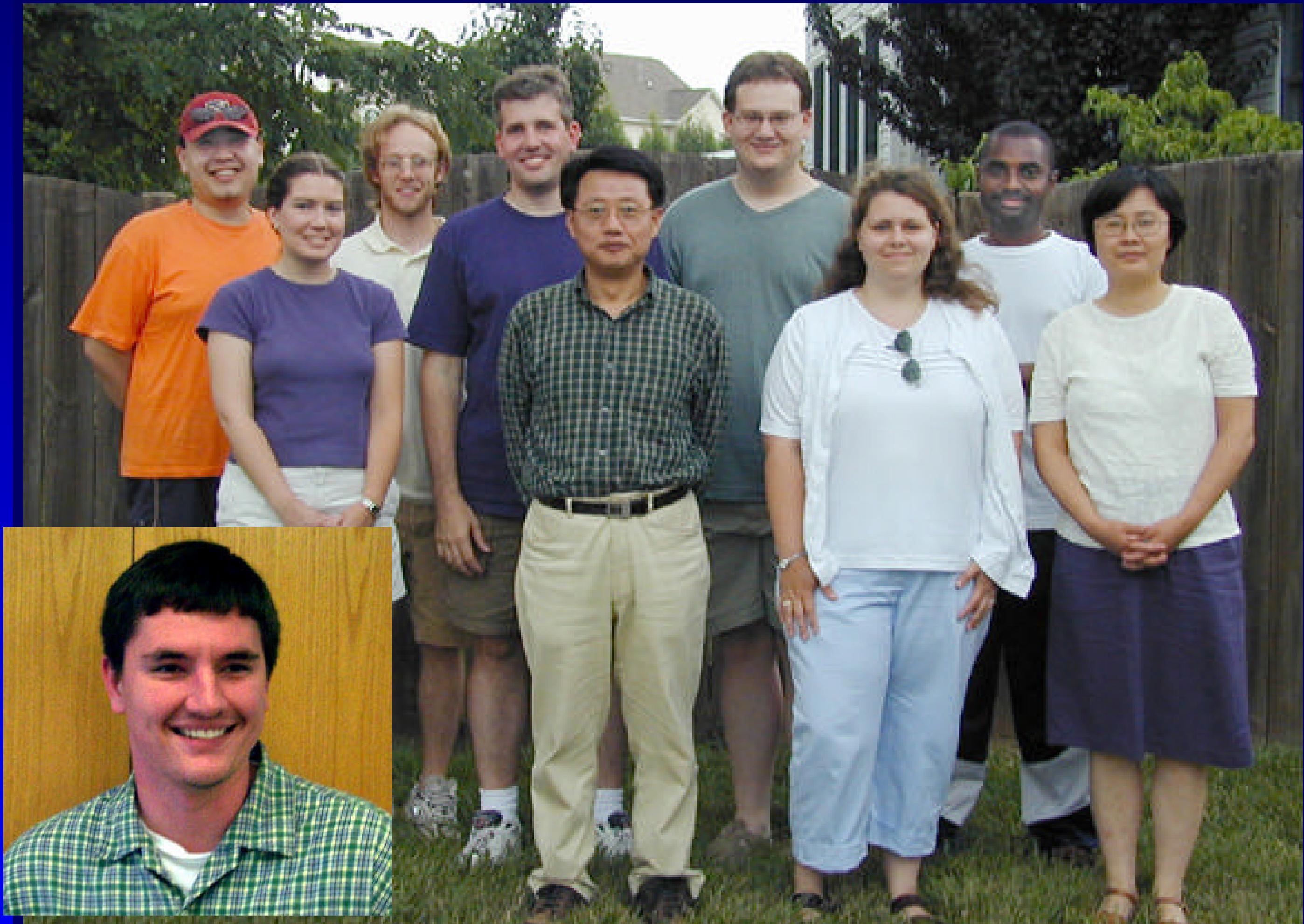
Particle Displacement



Conclusions & Questions

- Dependence on material
 - a-C:T is not an equilibrium system
 - Ring statistics ambiguous
 - Use hybridization, void volumes, Voronoi volumes
- Potential development needed
 - Long-range interactions
 - LJ not crucial
 - Screening is (environment-dependent bonding range)
 - Torsions useful (liquid C)
 - Strain energies
 - Oxygen, metals
 - Electrostatics?
- Accelerated dynamics
 - Parallel replica dynamics ? μs
 - Hyperdynamics? ? ms

Acknowledgements



**Art F. Voter, LANL
Blas Uberuage, LANL**

Dr. Oyeon Kum

**Brad Dickson
Janet Aremu-Cole
Todd Knippenberg
Aibing Liu
Michael Mury
Pam Piotrowski
Suleiman Oloriegbe**

Yang Li

DoD

SC CHE

**Postdoc position available: TB, electrostatics, or
potential development experience**

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