

Liquid-vapor coexistence and critical point of Mg_2SiO_4 from *ab-initio* simulations

JP Townsend¹, G Shohet², K Cochrane¹

¹ Sandia National Laboratories, Albuquerque, NM

² Department of Aeronautics & Astronautics, Stanford University, Stanford, CA



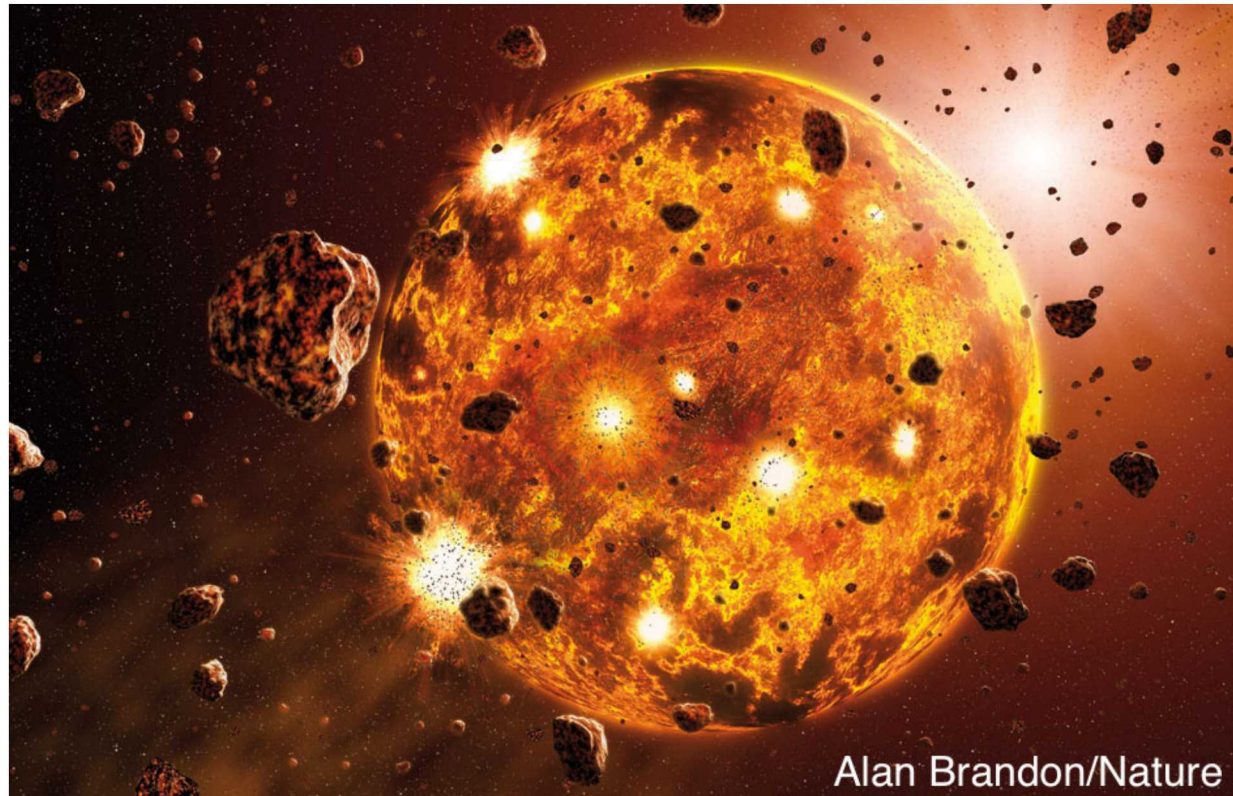
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND NUMBER

Goal: Advance planetary accretion models

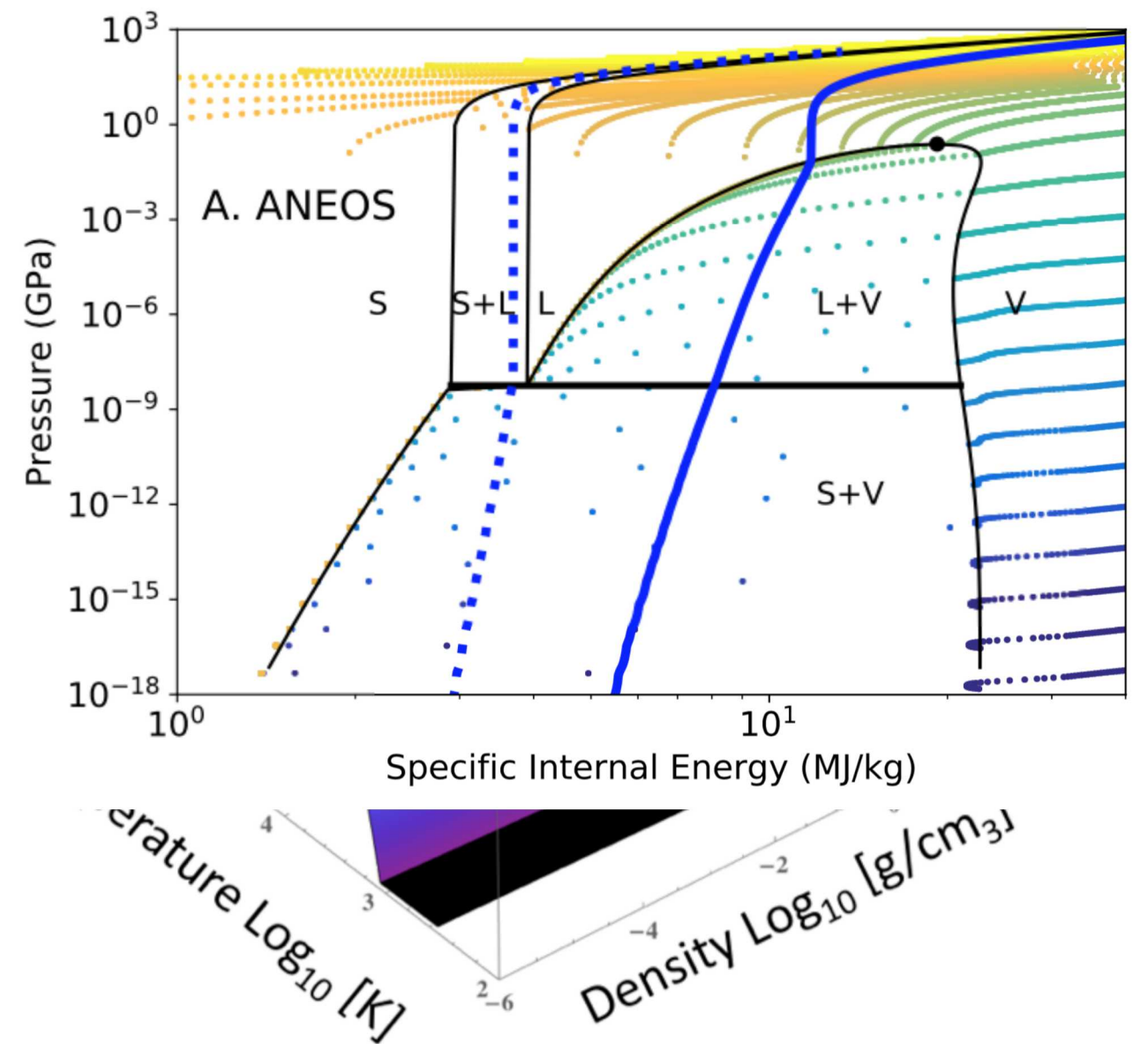


Critical behavior is essential to accretion process

Goal: Advance planetary accretion models



Extant EOS models rely on simplified models



Critical behavior of silicates *entirely unknown!*

Computational Approach

Simplest EOS with a critical point:

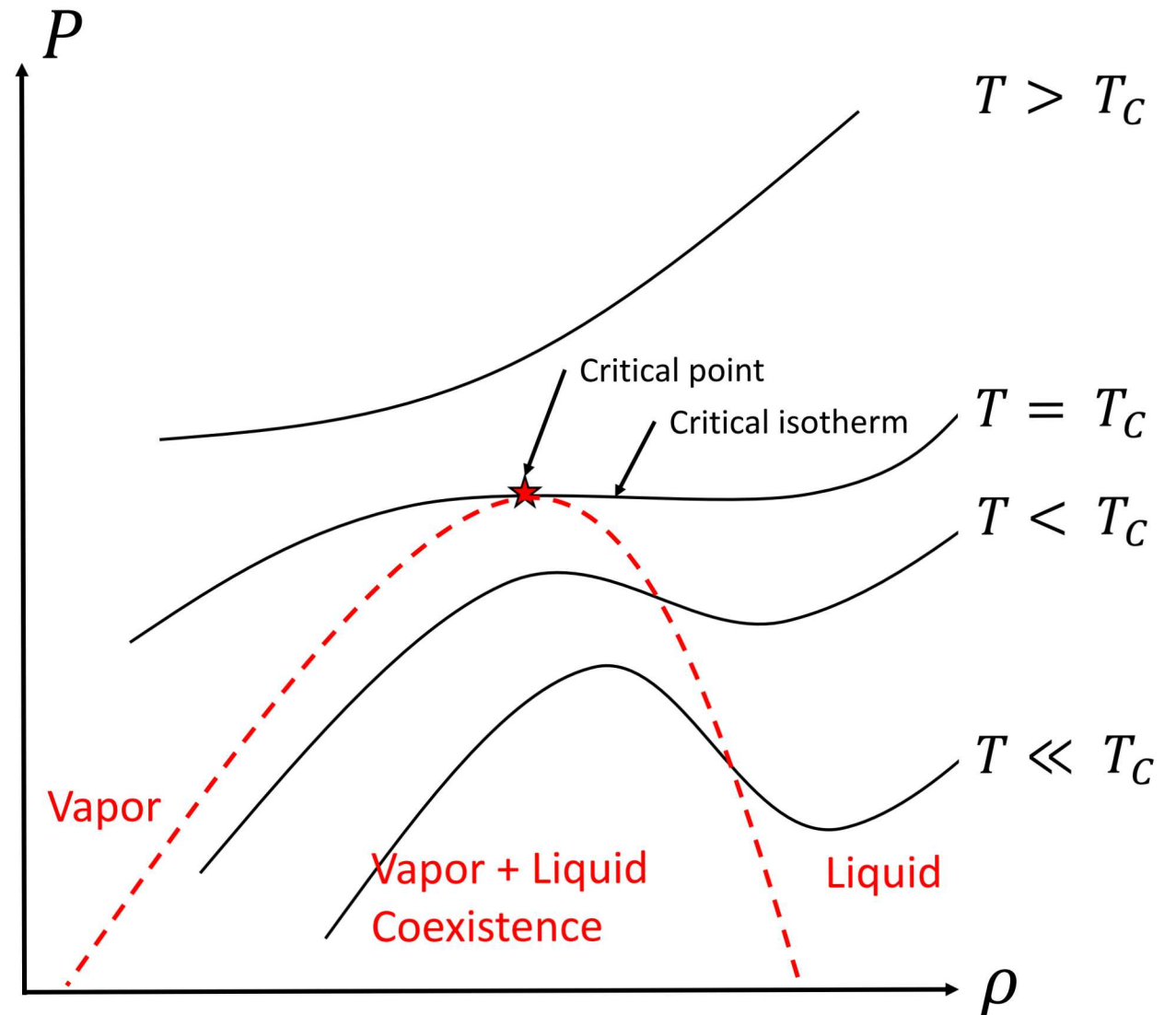
$$P(\rho, T) = a(T) + b(T)\rho + c(T)\rho^2 + d(T)\rho^3$$

At the critical point:

$$\left(\frac{\partial P}{\partial \rho}\right)_T = \left(\frac{\partial^2 P}{\partial \rho^2}\right)_T = 0$$

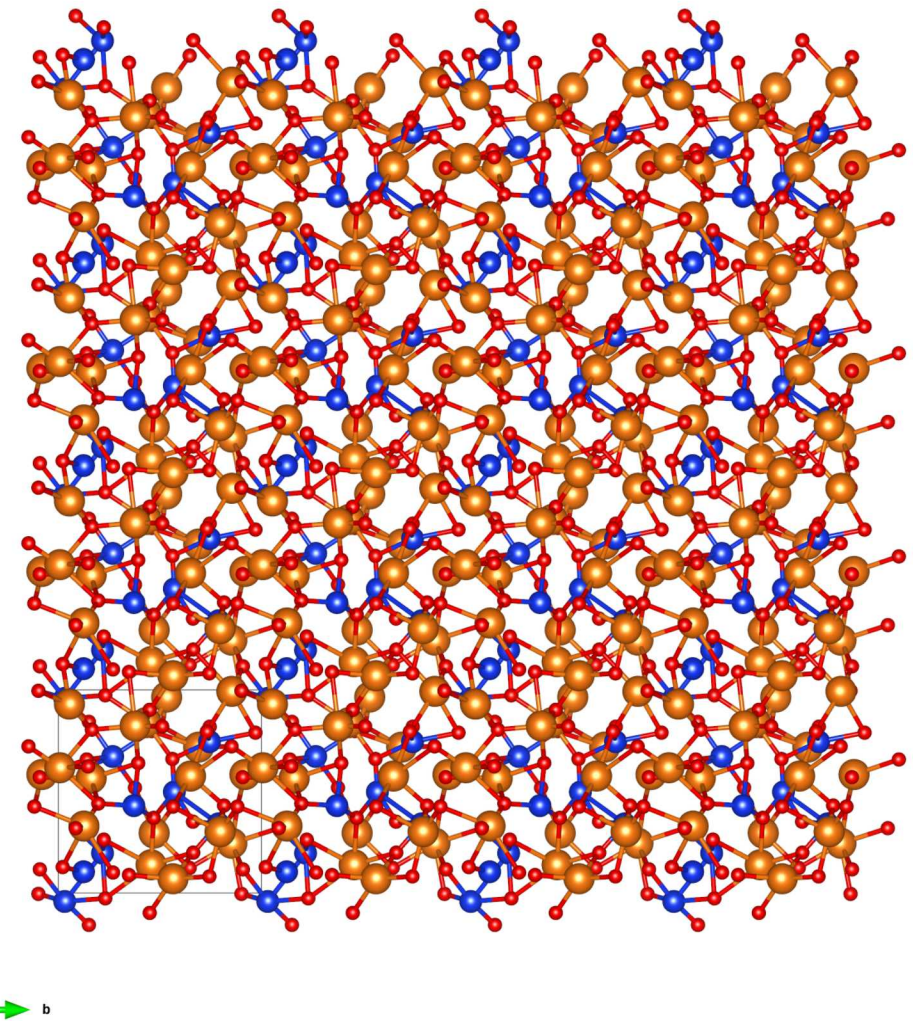
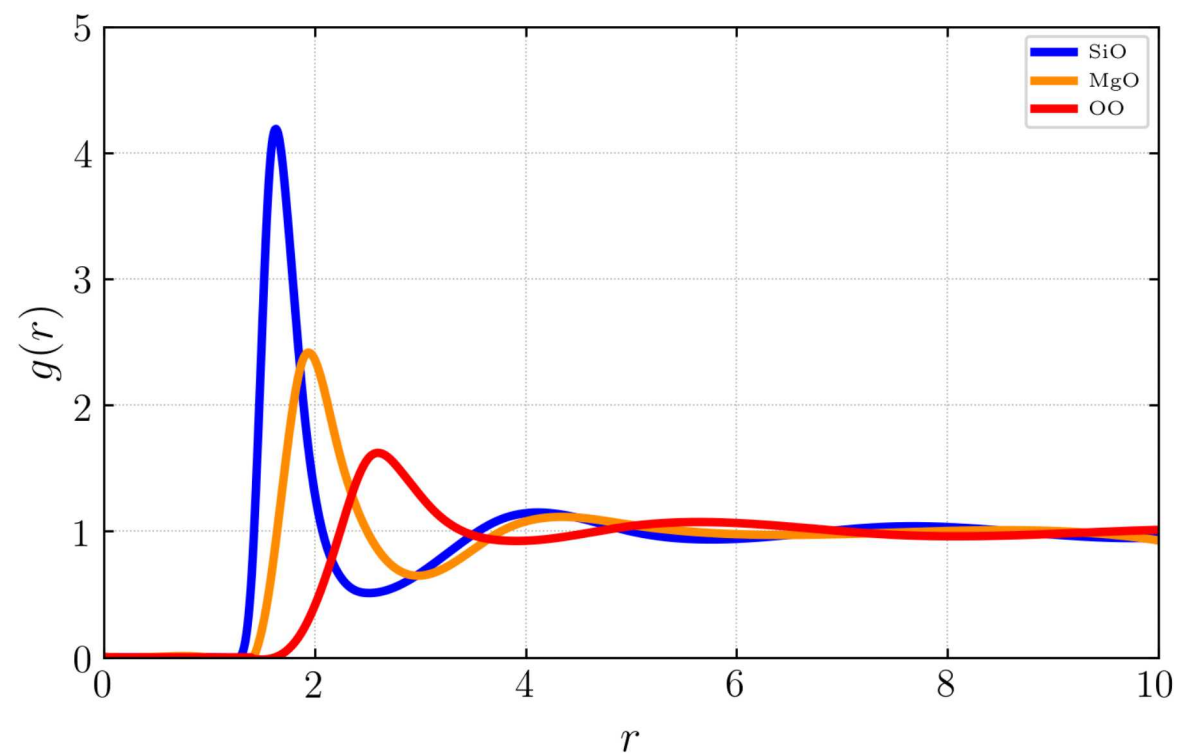
MD calculations:

- **VASP + PAW's**
- **Mermin functional**
- **NVT with N=56/112**
- **PBE xc functional**



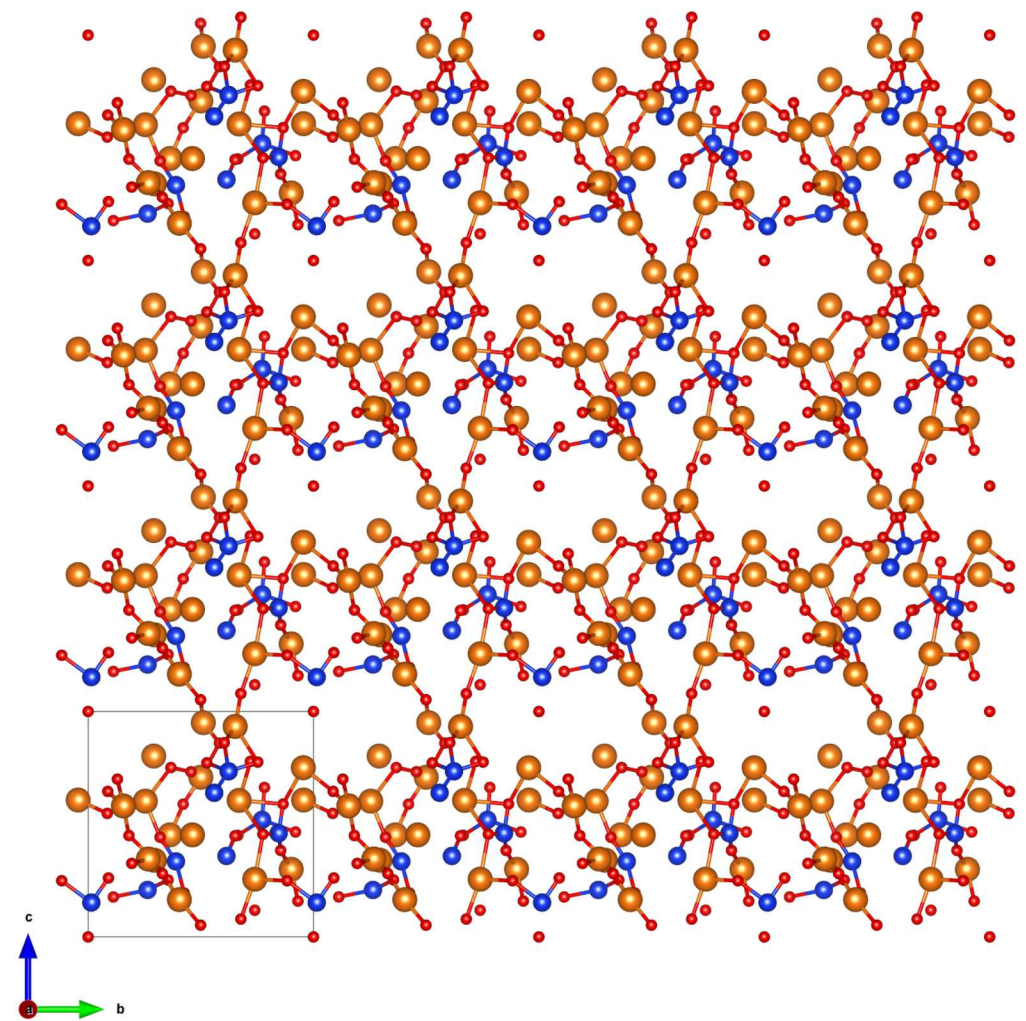
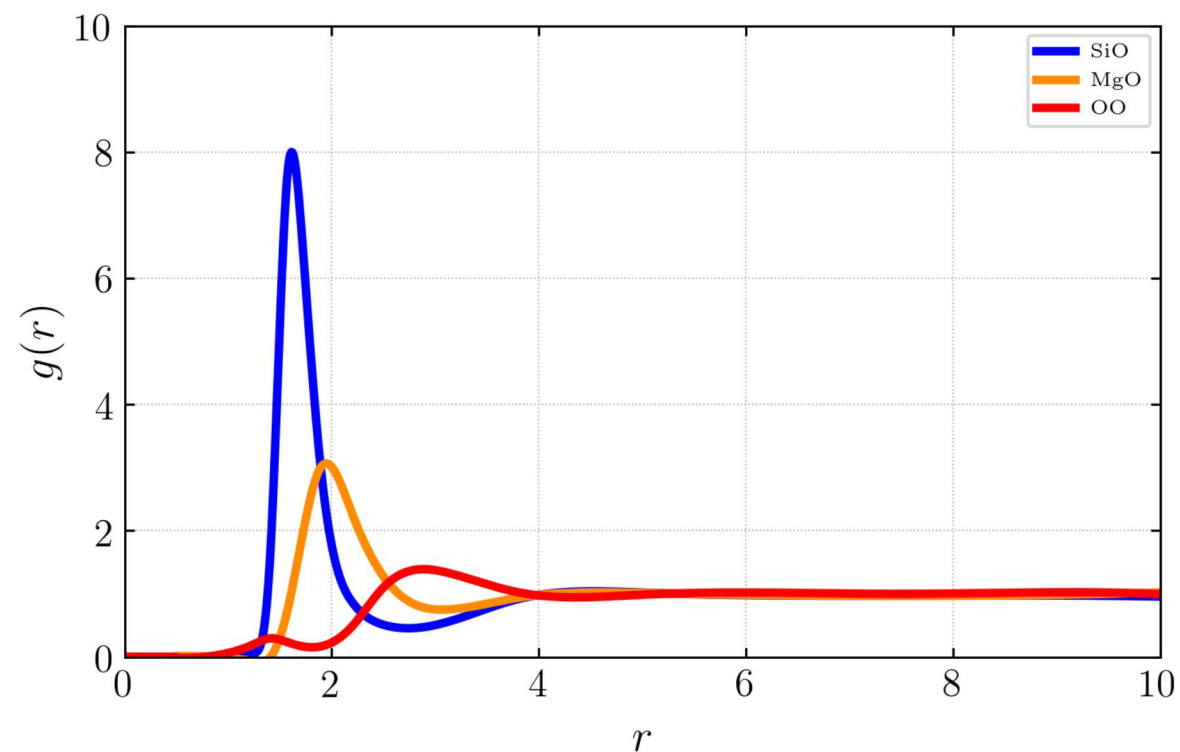
Continuous structural evolution

$\rho = 3.22 \text{ g/cm}^3$
 $T = 6000 \text{ K}$



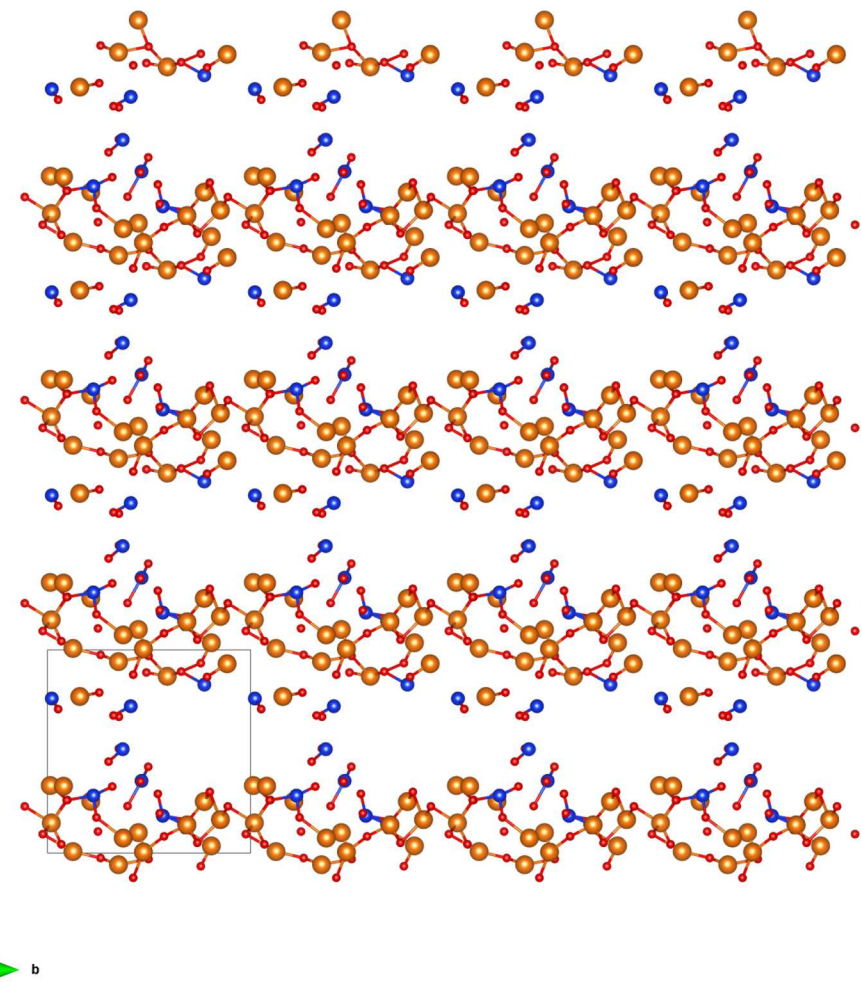
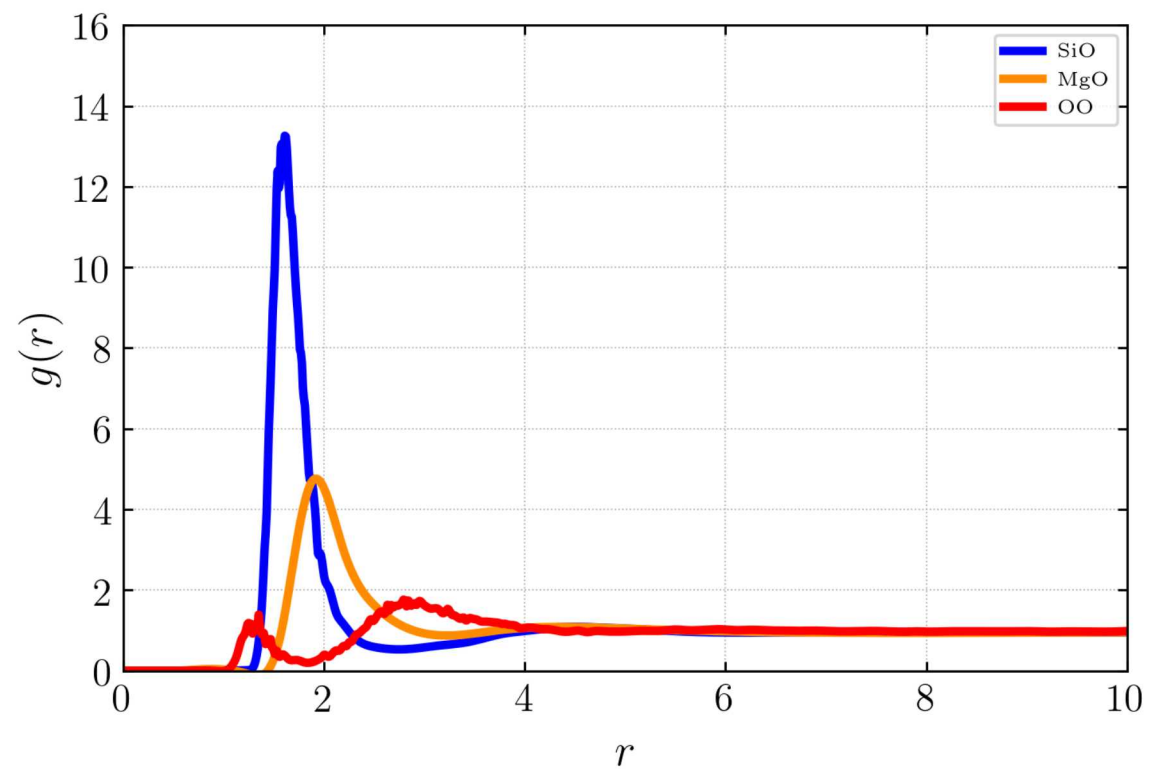
Continuous structural evolution

$\rho = 1.22 \text{ g/cm}^3$
 $T = 6000 \text{ K}$



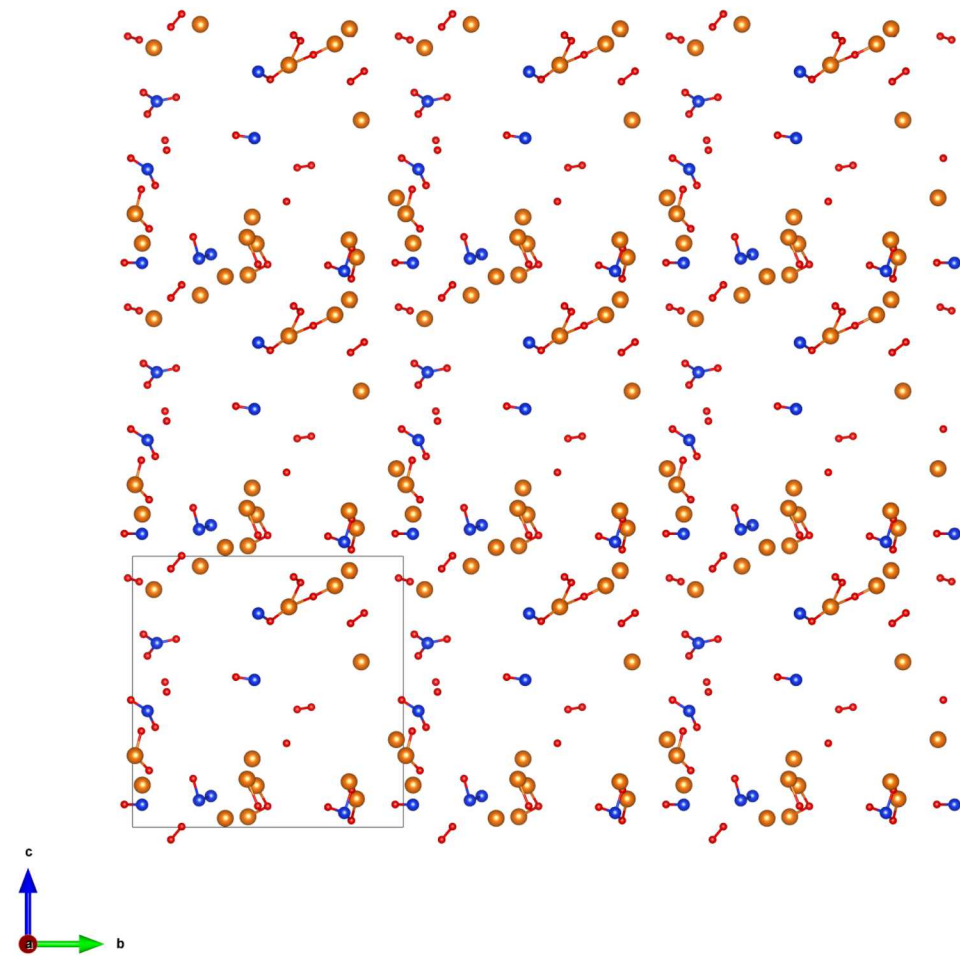
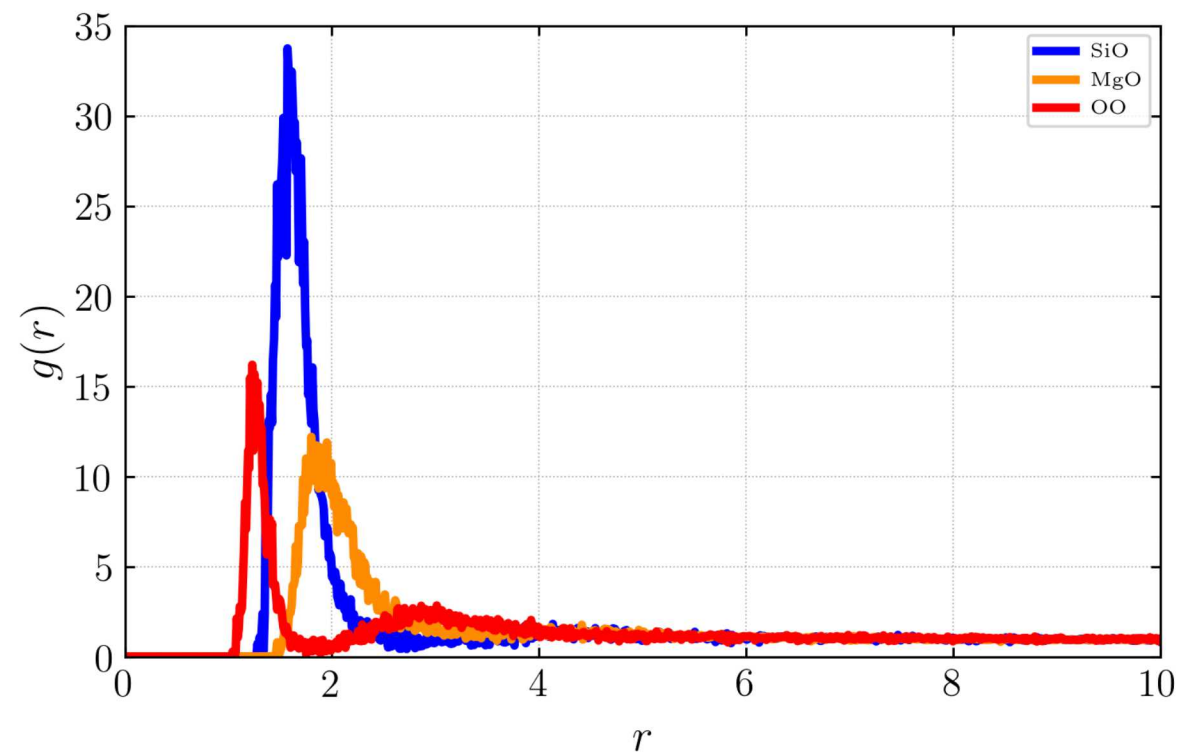
Continuous structural evolution

$\rho = 0.72 \text{ g/cm}^3$
 $T = 6000 \text{ K}$

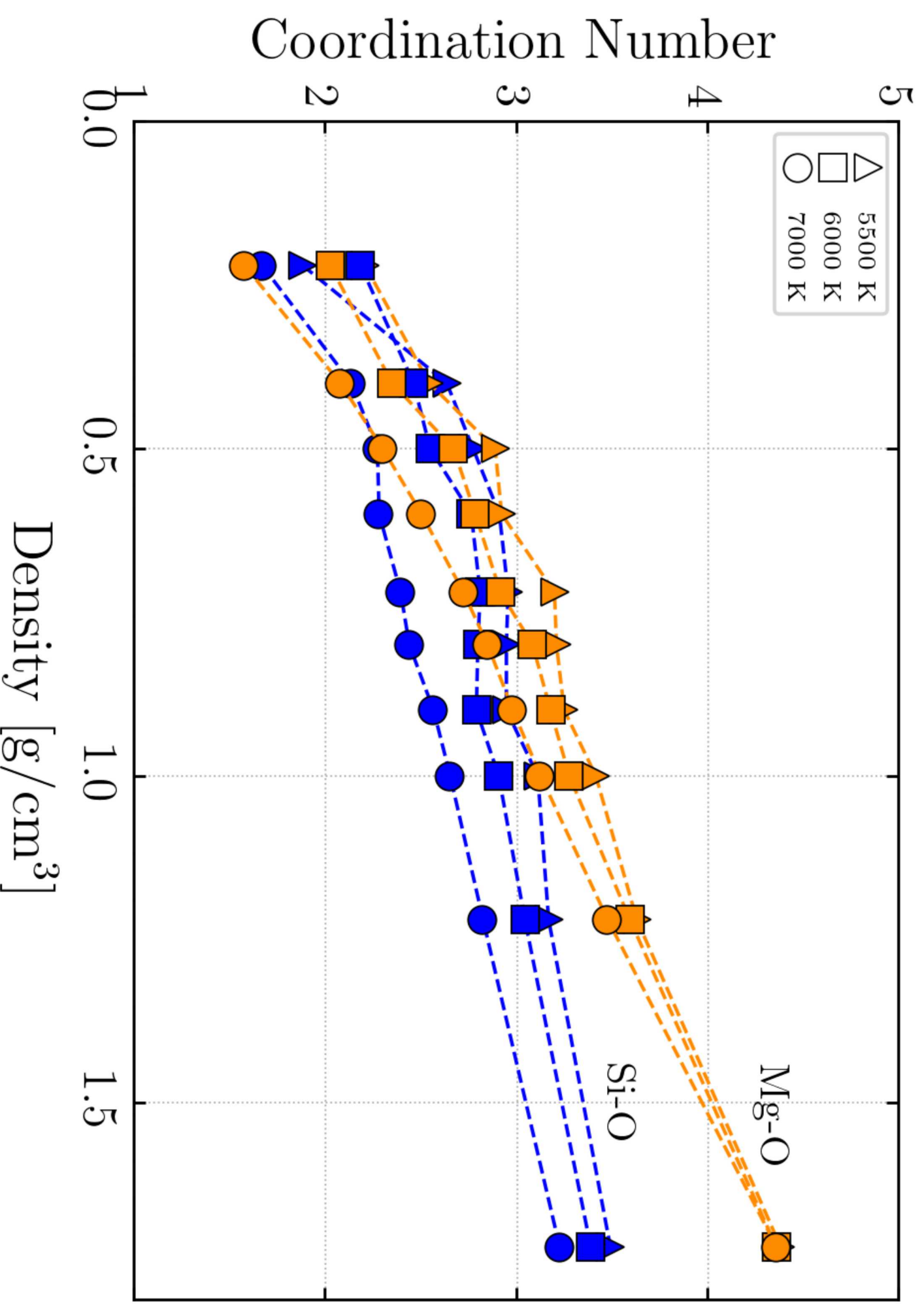


Continuous structural evolution

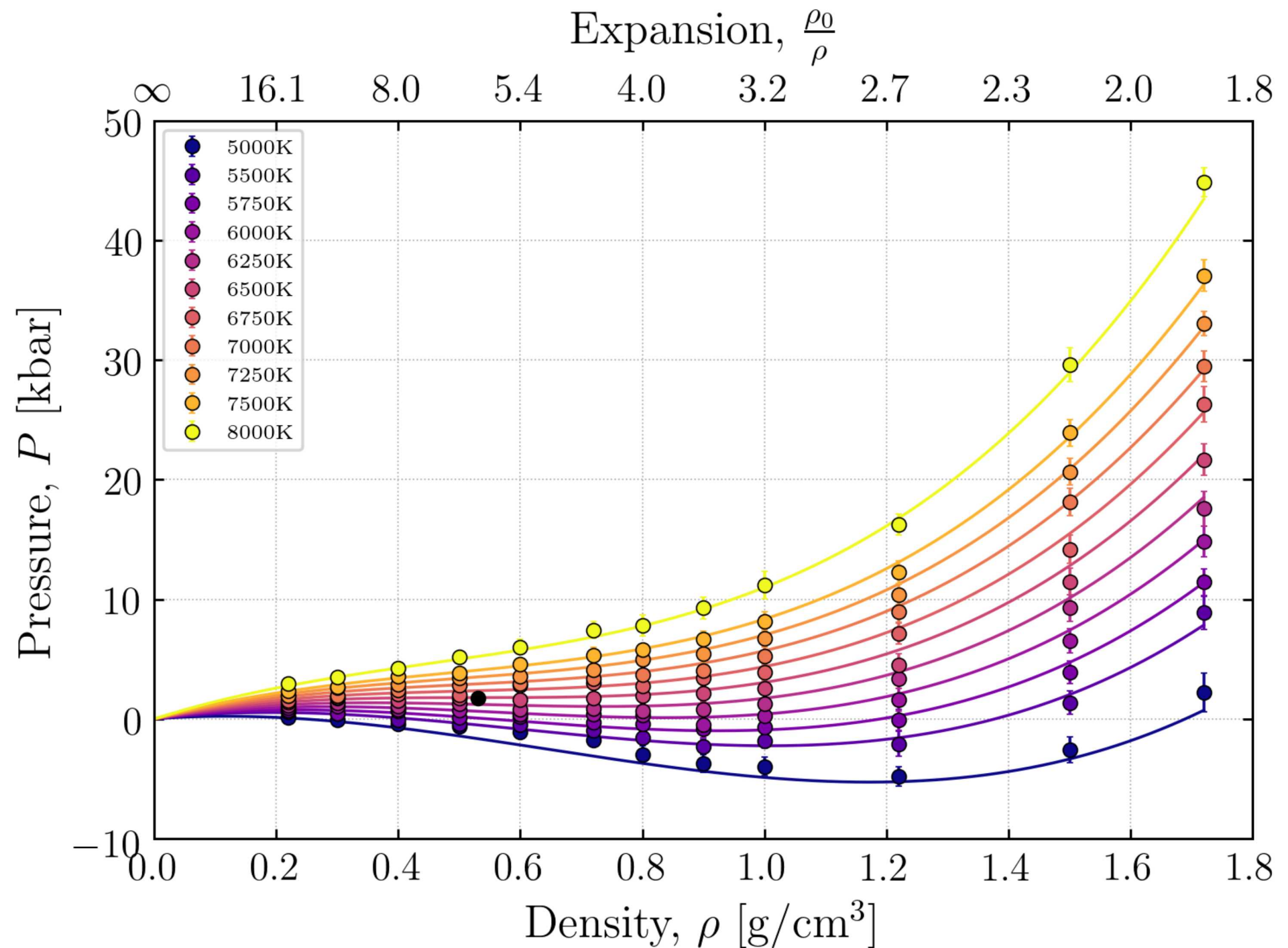
$\rho = 0.22 \text{ g/cm}^3$
 $T = 6000 \text{ K}$



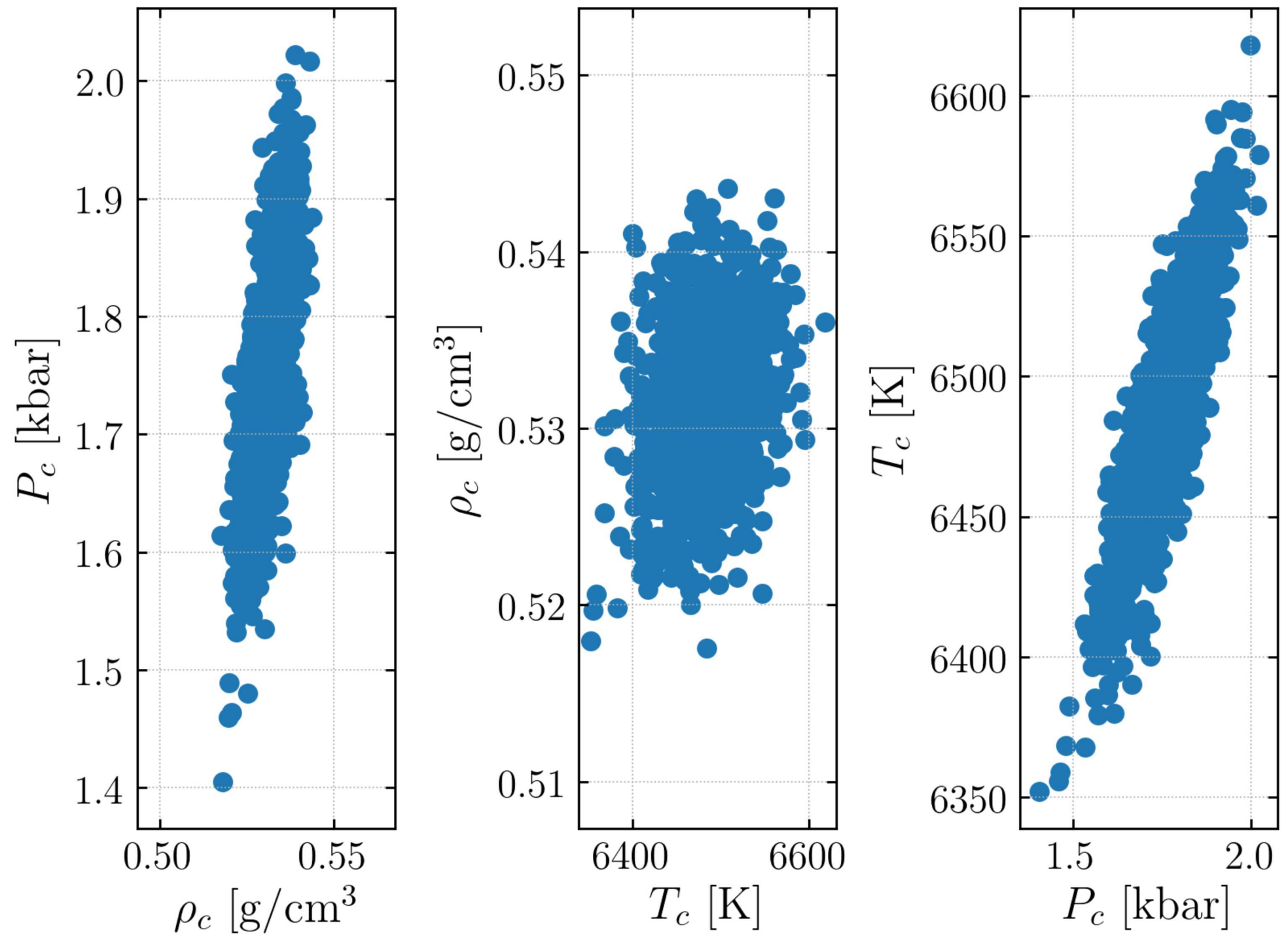
Continuous structural evolution



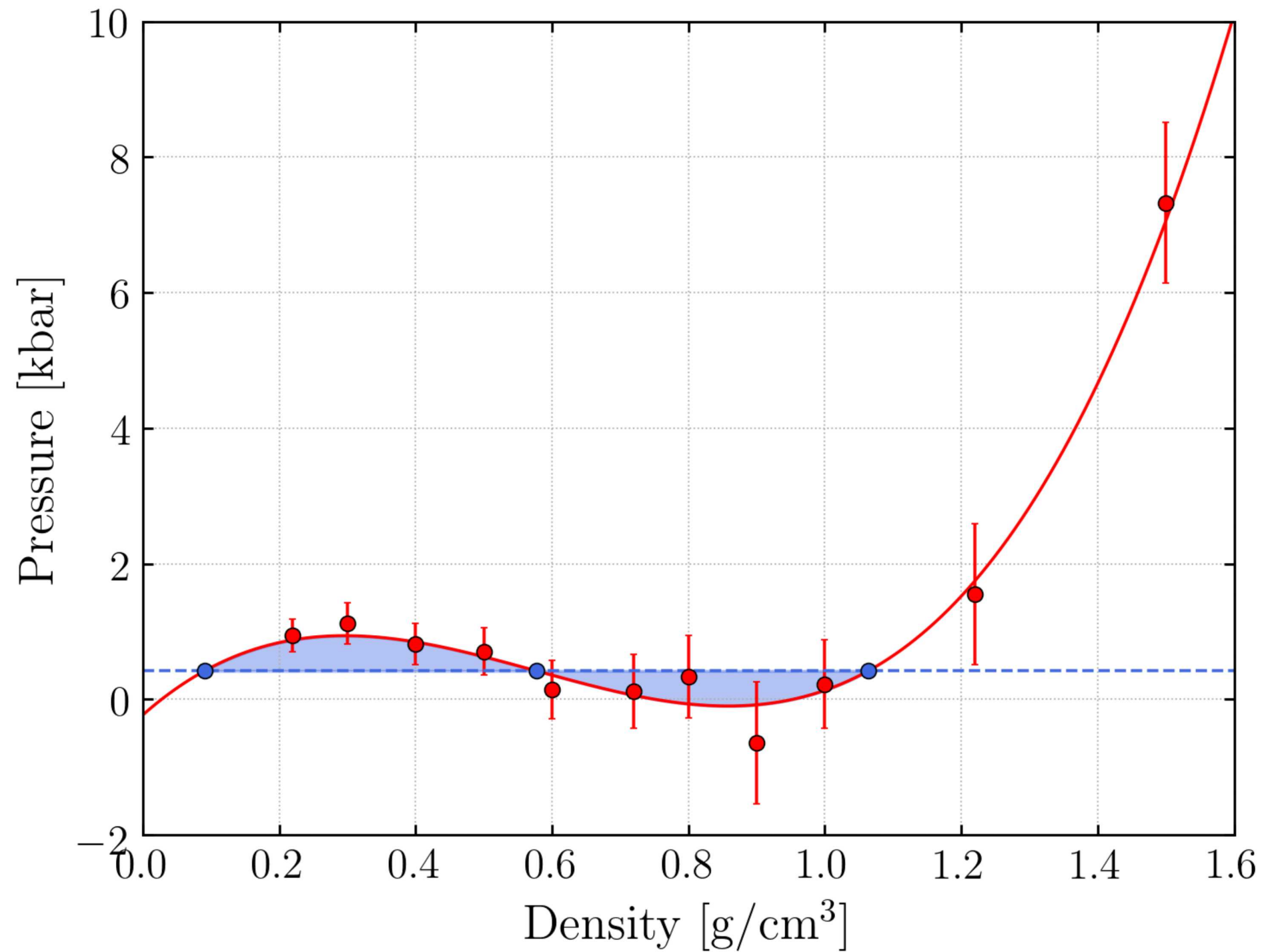
Critical point estimation



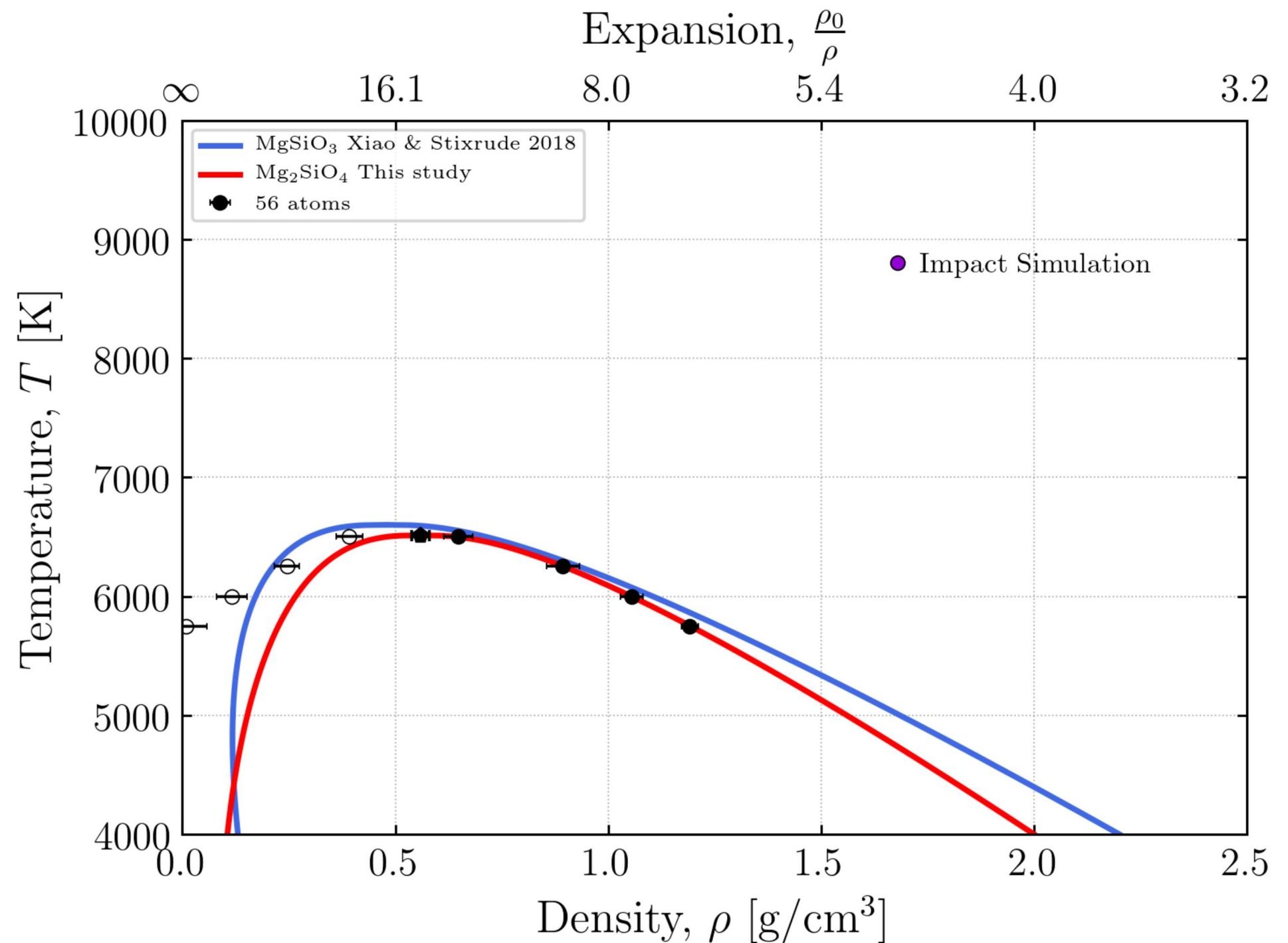
Critical point estimation



Maxwell construction



Coexistence curve



Summary

- **NVT DFT-MD calculations span 0.22-3.22 g/cc
5000-8000 K**
- **Critical point estimated from EOS**
- **RG-coexistence phase boundaries**
- **Incongruent vaporization**