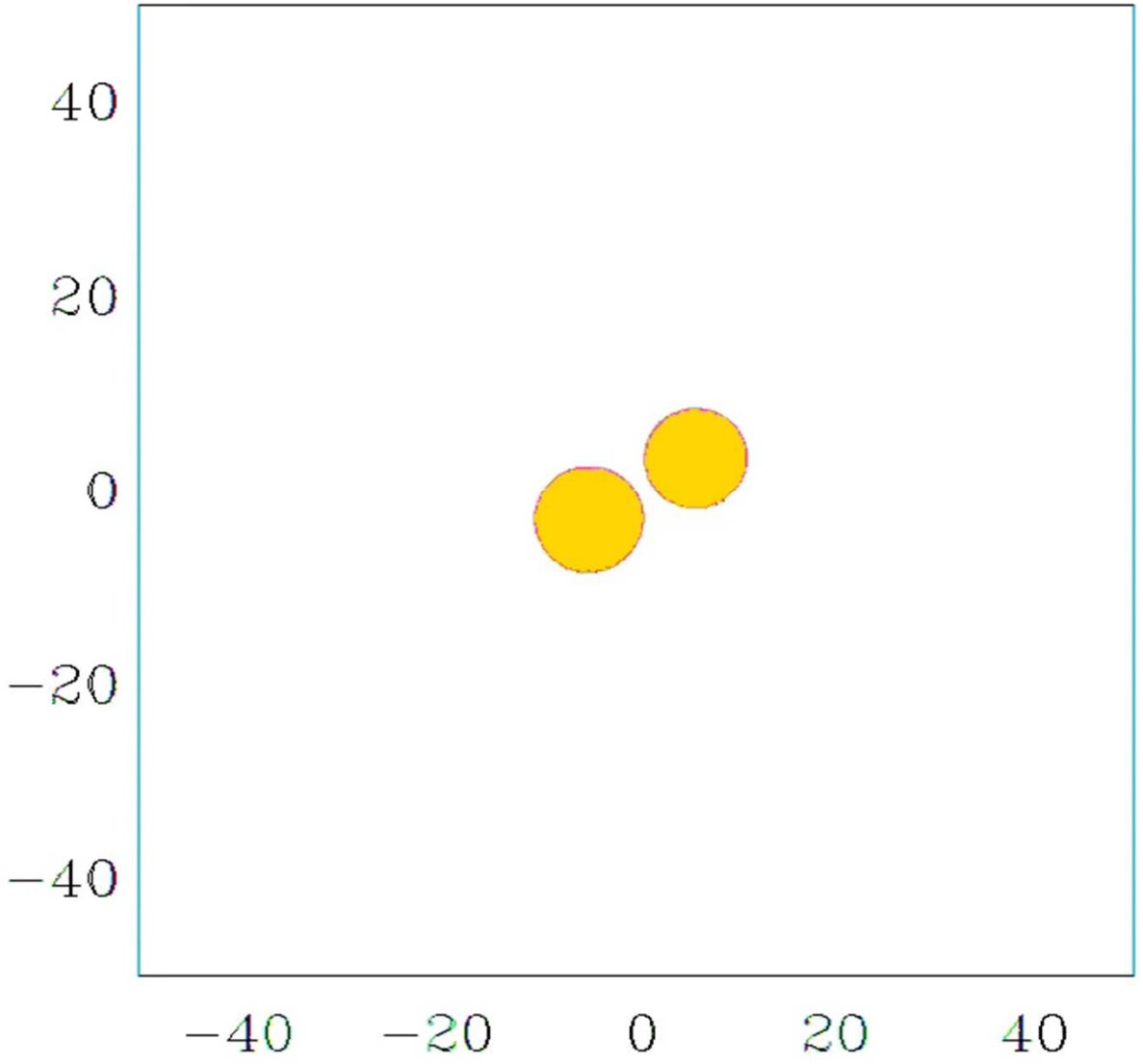
The year is 100,000,000. (The age of the Earth and of the solar system, is ~ 4,568,000,000)



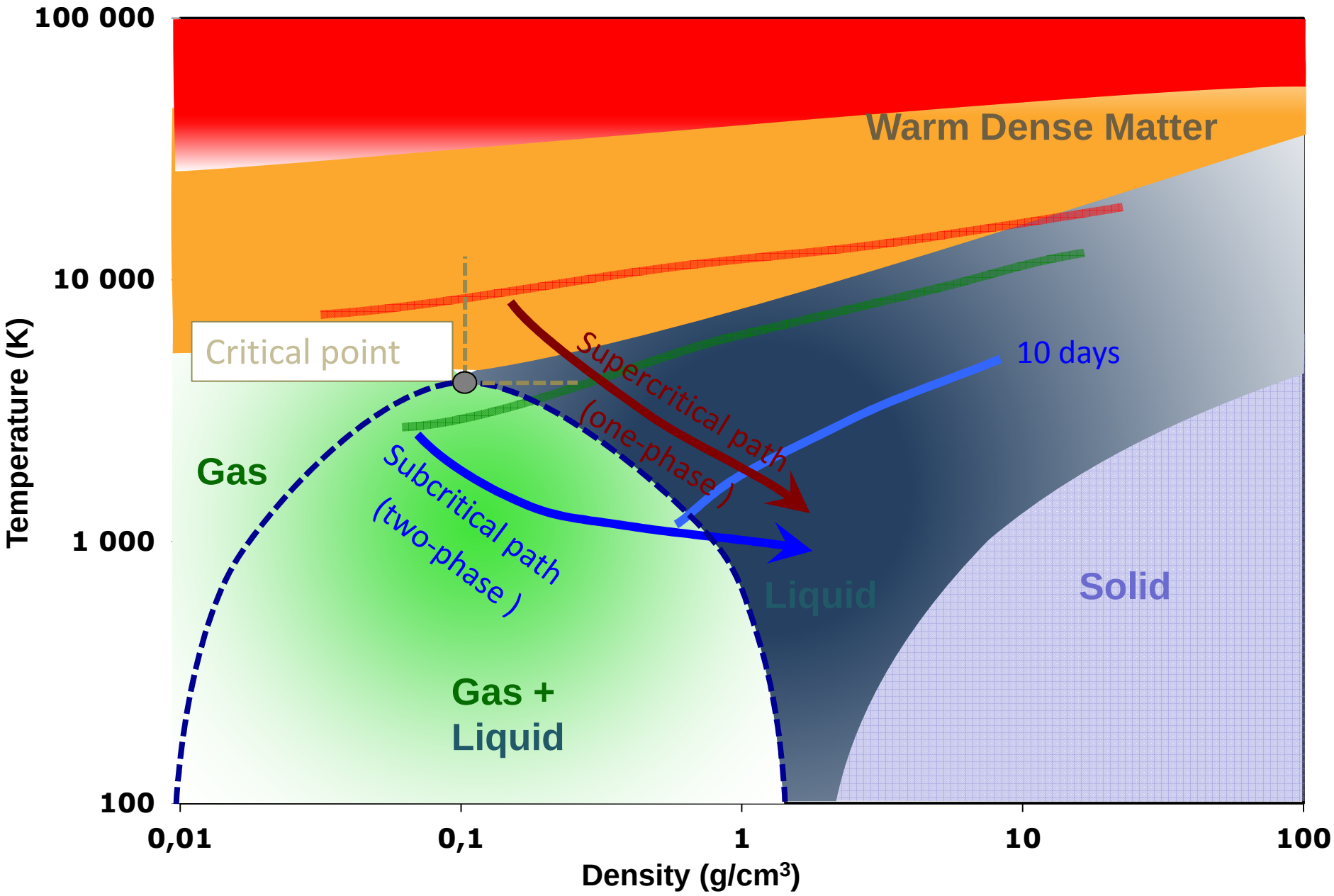
ABINIT
and
the formation of the Moon

Razvan Caracas

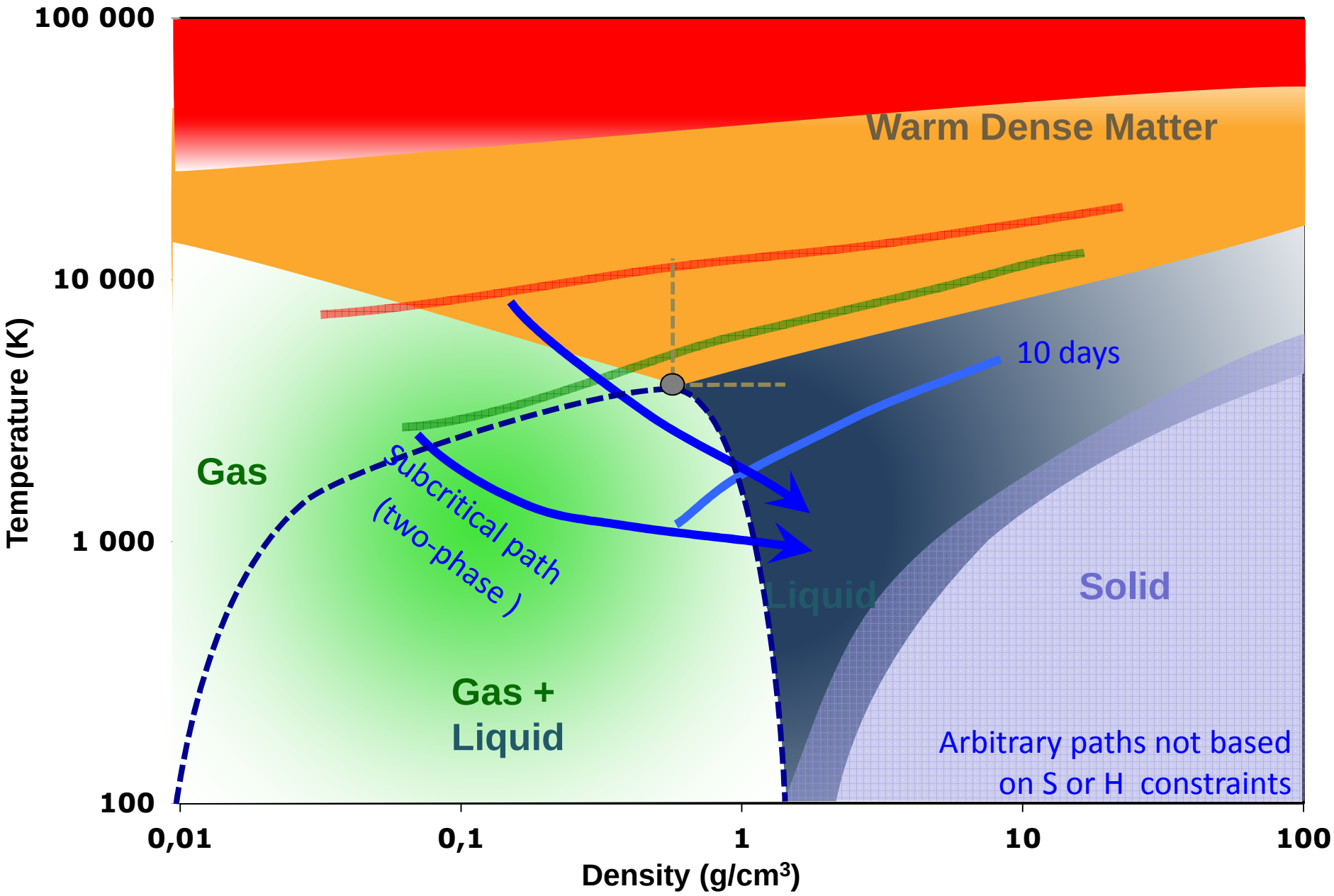
CNRS, ENS de Lyon

Evolution and condensation of the proto-lunar disk

subcritical or supercritical? this is the question!

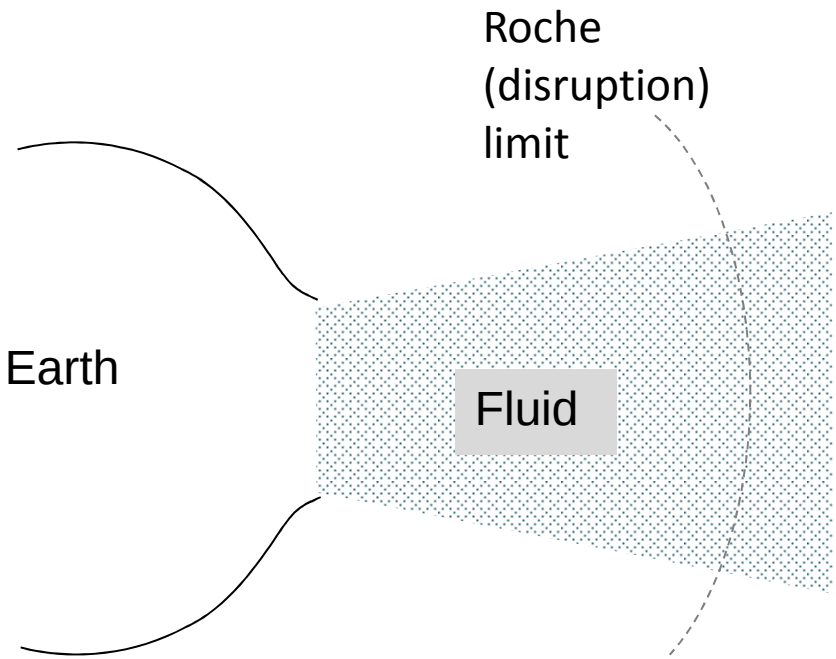


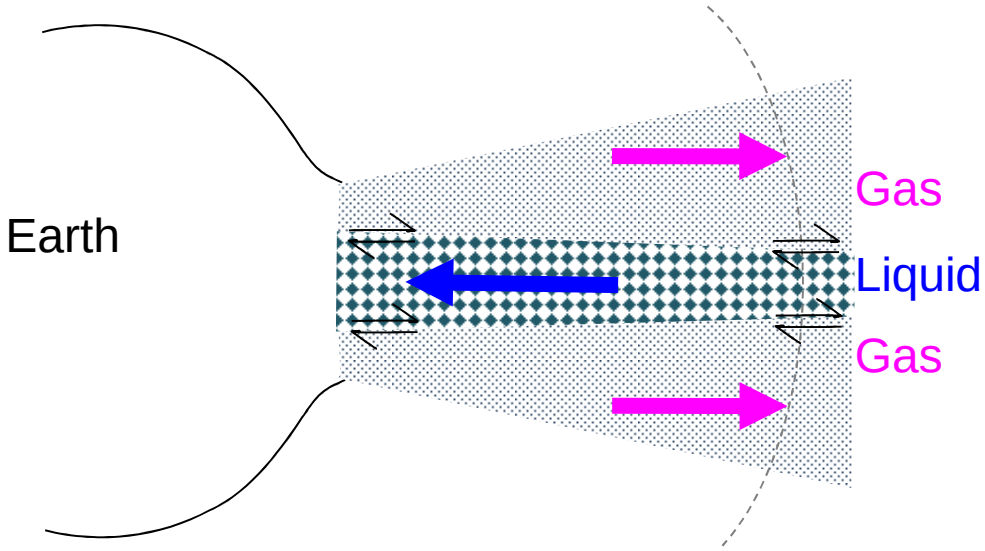
subcritical or supercritical? this is the question!



Different dynamical regimes of the disk after the impact

Exchange of angular momentum
by liquid – vapor friction

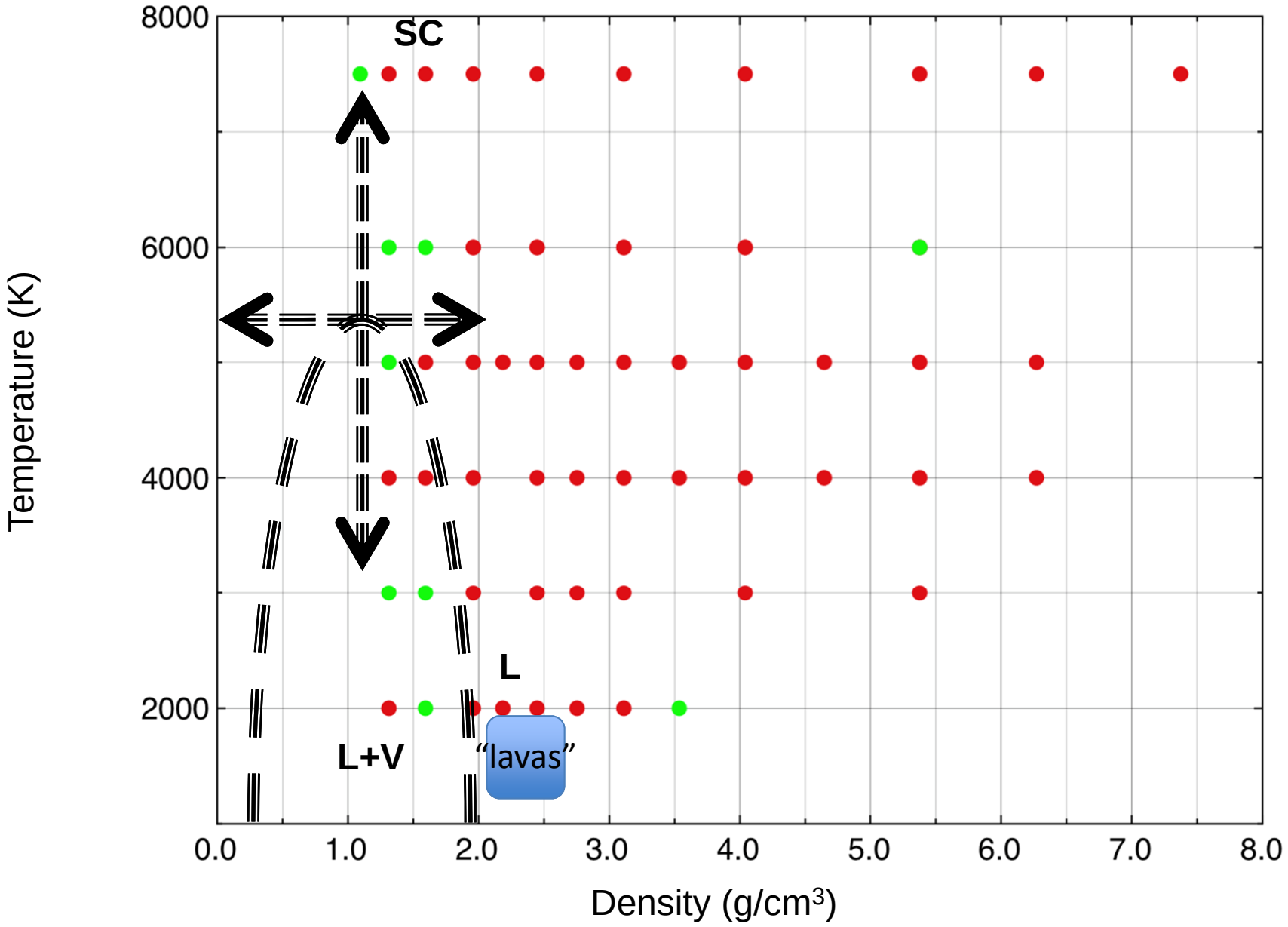




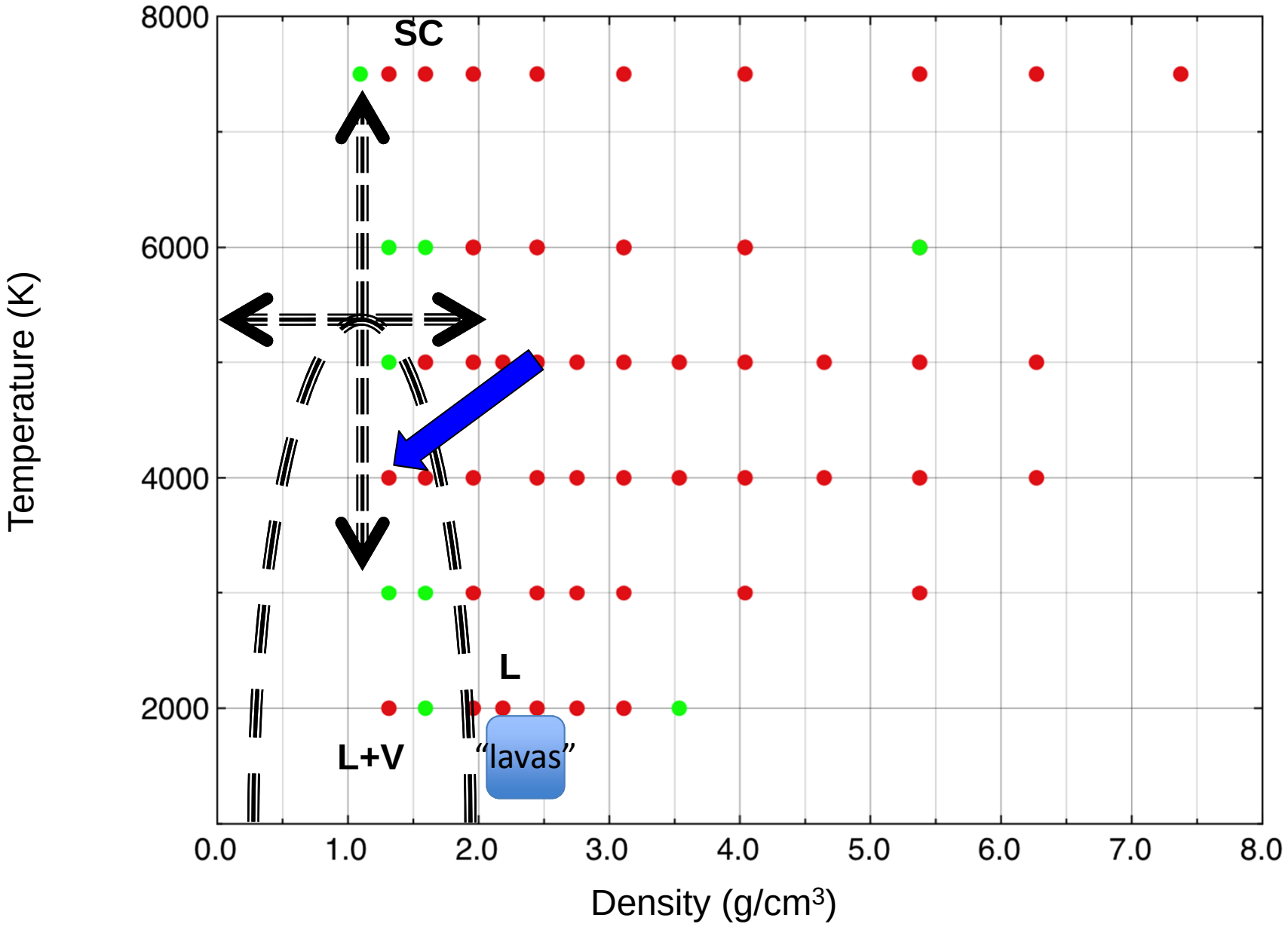
HOTTER disk
Supercritical
one-phase

COLDER disk
Subcritical
two-phase

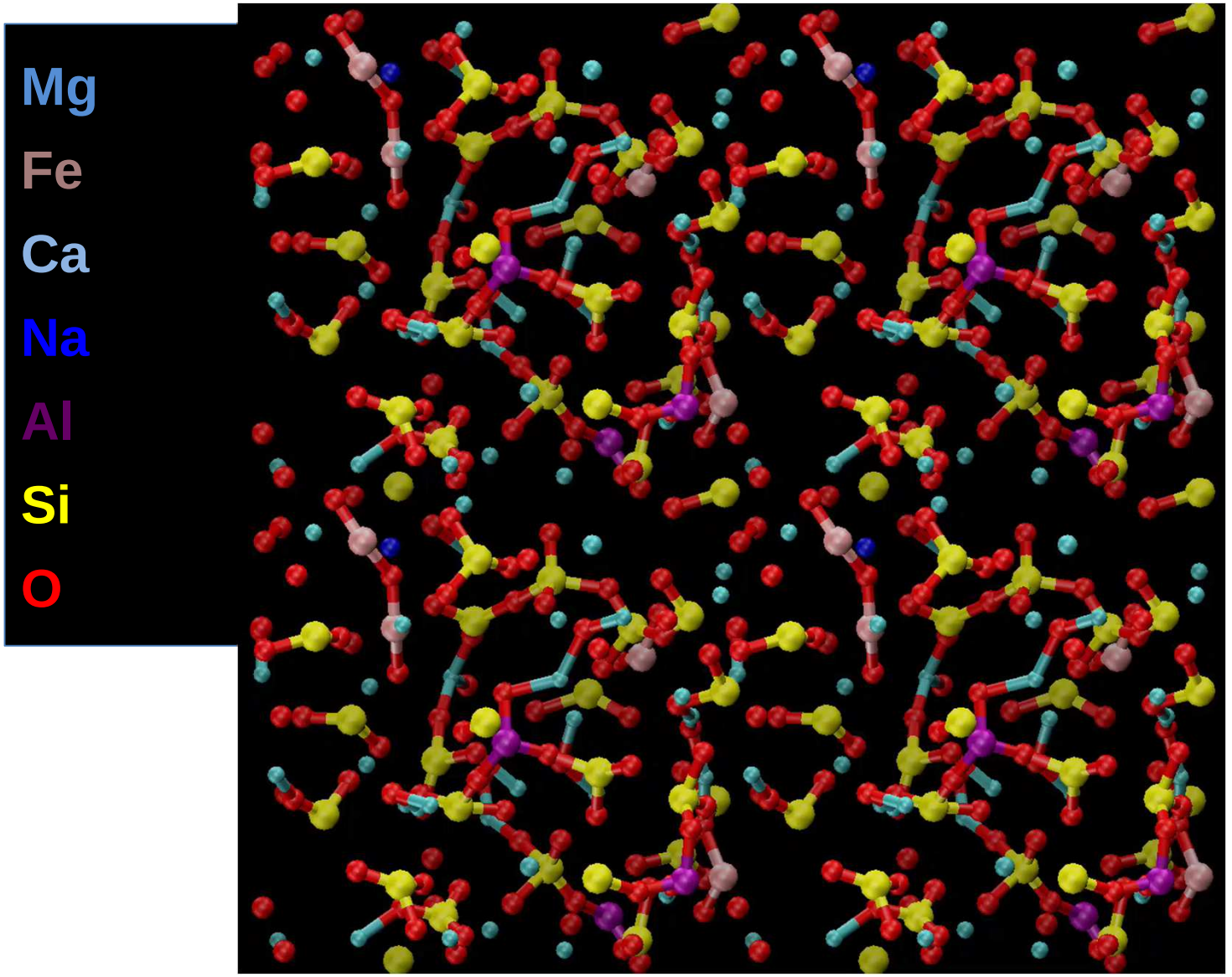
RECONSTRUCTING THE GIANT IMPACT - pyrolite melts



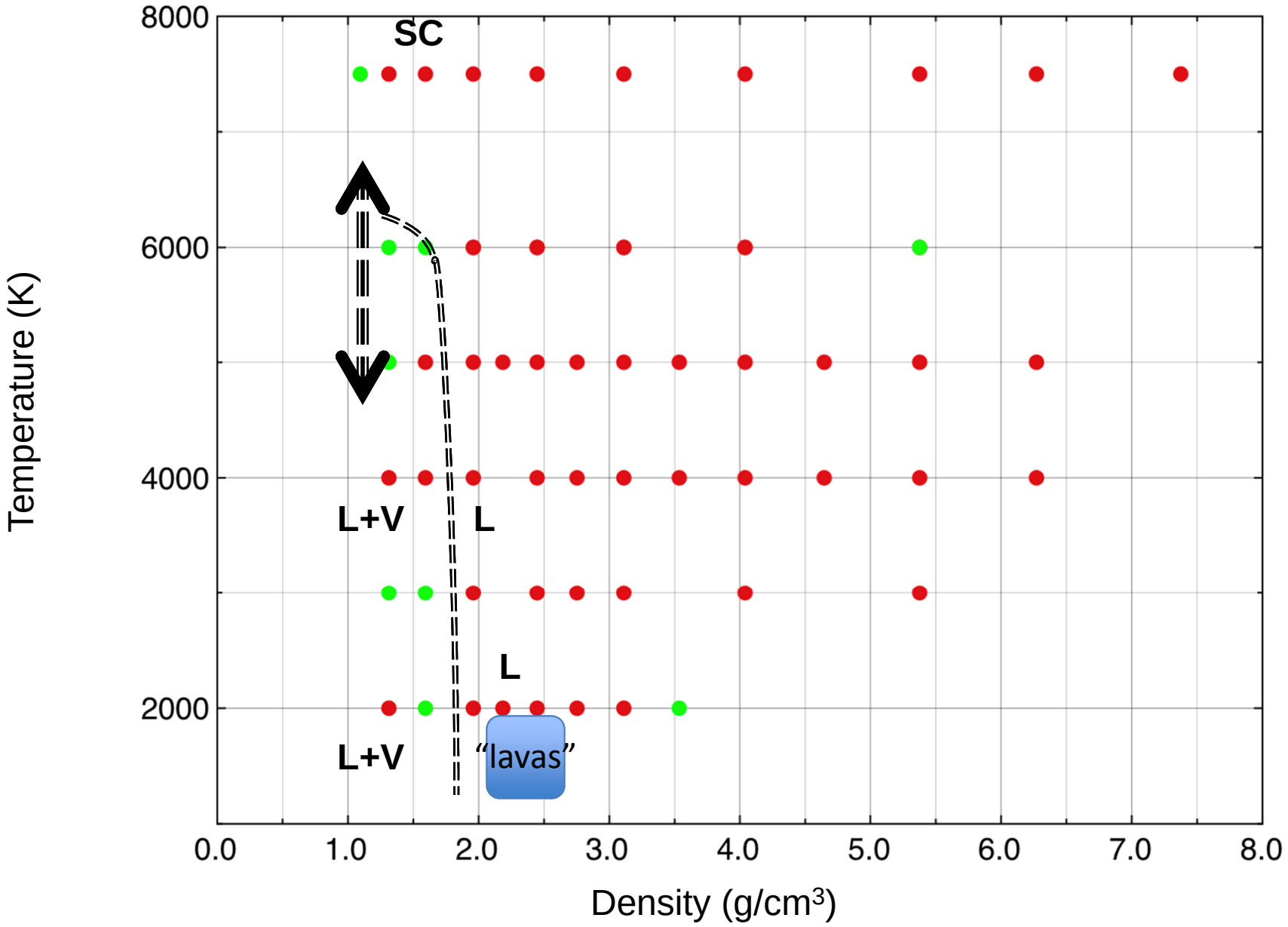
RECONSTRUCTING THE GIANT IMPACT - pyrolite melts



$\rho = 1.313\ g/cm^3$
T = 4000K



RECONSTRUCTING THE GIANT IMPACT - pyrolite melts



TO DO list:

1. (Thermo)dynamics from (PI)MD simulations
   - Compute the supercritical domes
   - Place the supercritical points
   - Build the liquid/vapor equilibrium “curves”
   - Equation of states of the liquid
   - Thermodynamic properties of the liquid and gas
   - Speciation in the vapor phase
   - Isotope and chemical partitioning functions
2. Electronic/optical properties
   - GW calculations on atomic clusters of the gas phase
   - GW calculations on the liquid phase (snapshots)
   - Optical signatures for identification