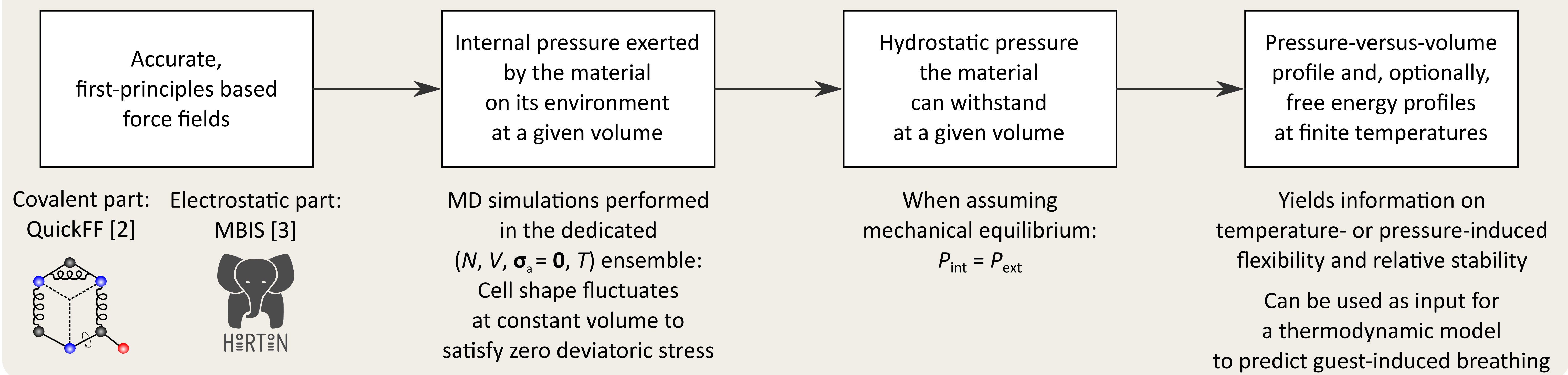


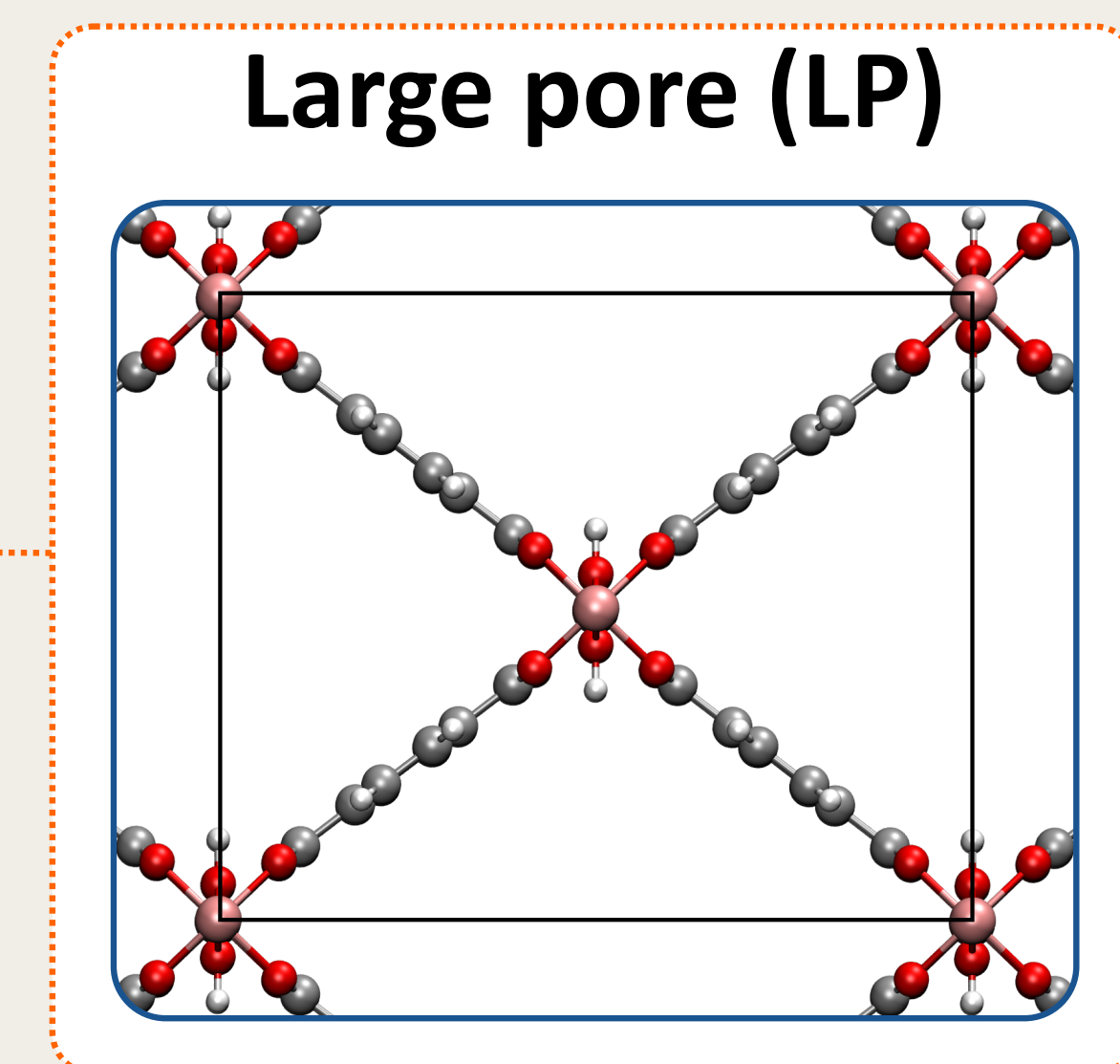
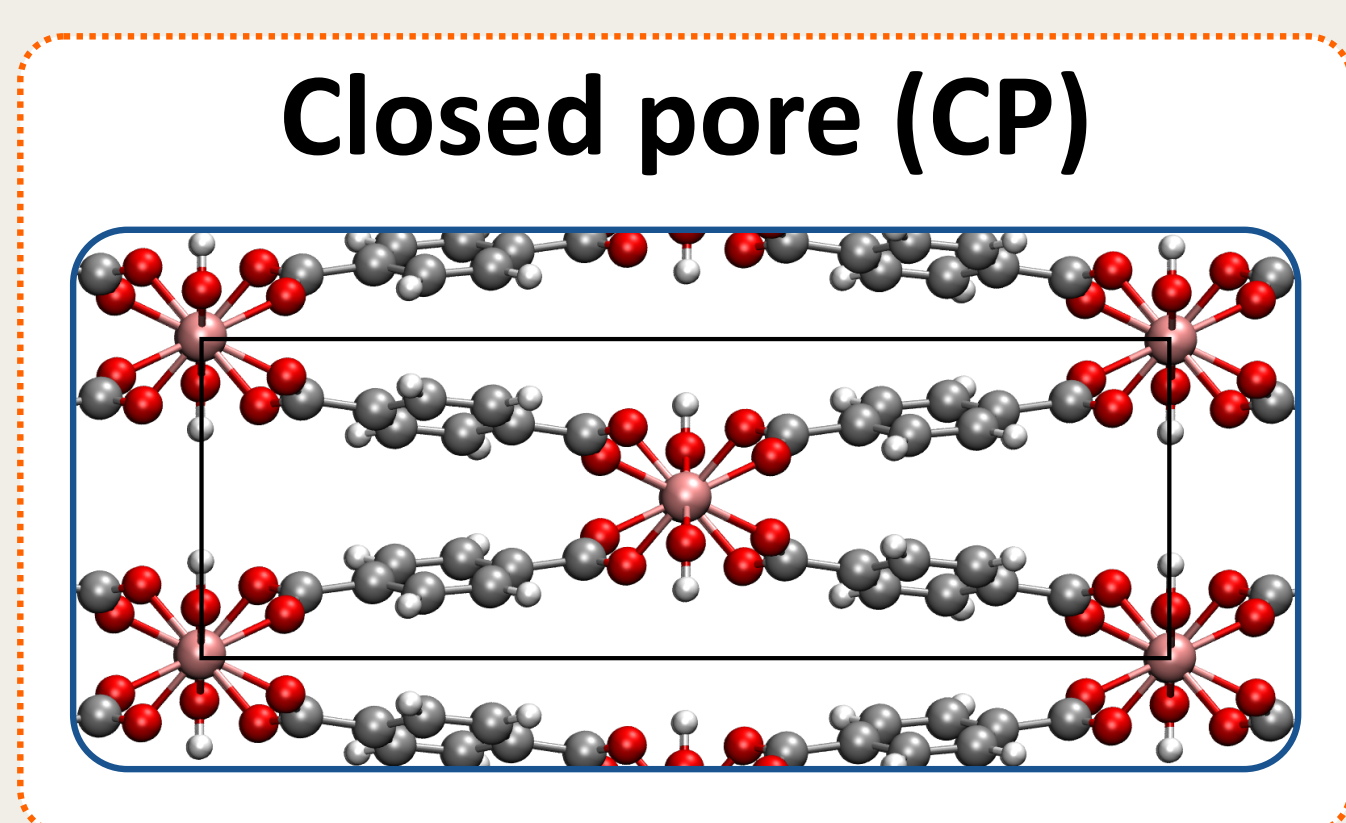
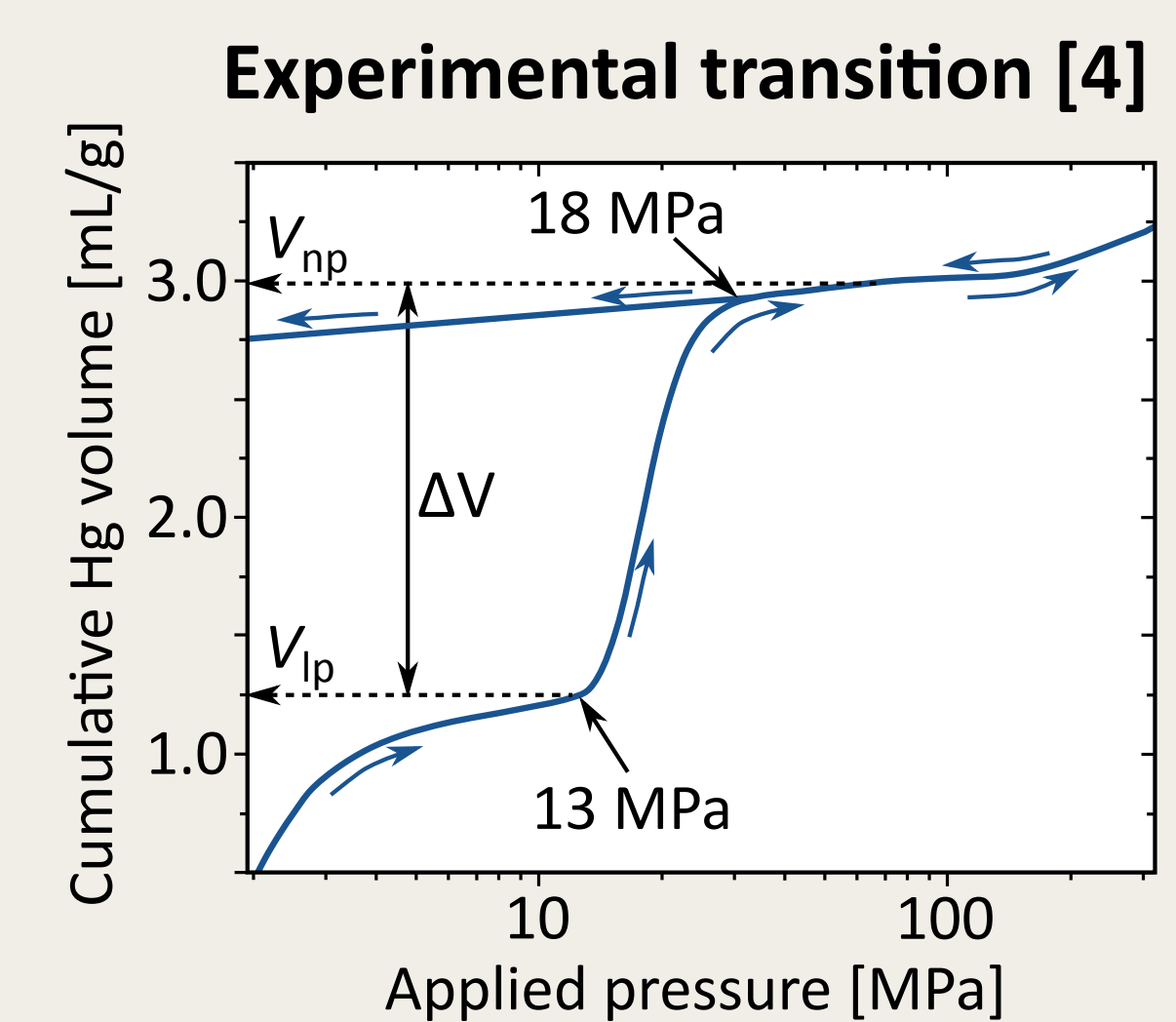
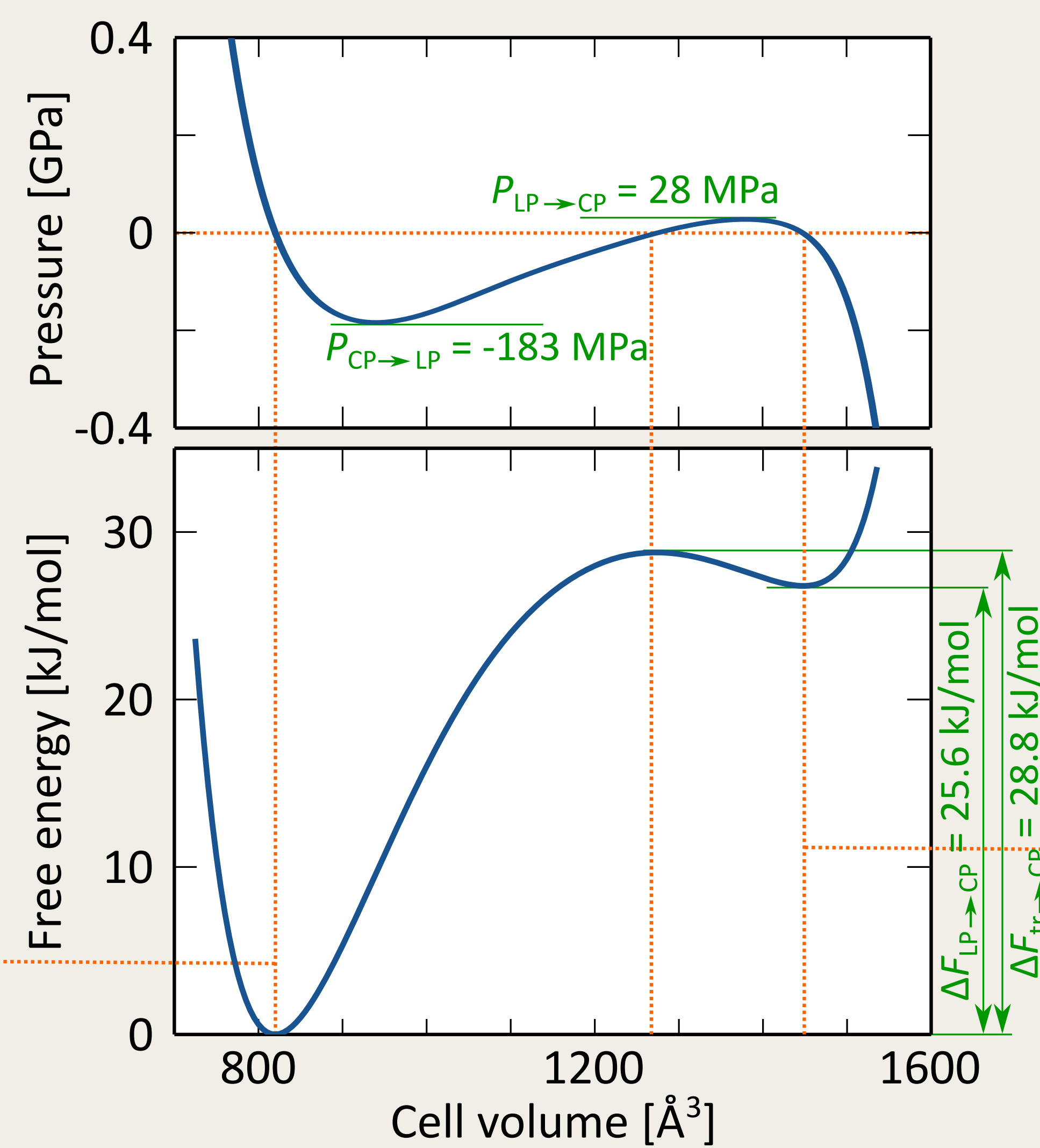
## Our thermodynamic protocol [1]



## Pressure-induced breathing in the flexible MIL-53(Al) at 300 K [1]

MIL-53(Al) breathes between a CP and a LP phase, which can be induced by pressure, temperature, and guest adsorption.

Within our approach, the experimental LP  $\rightarrow$  CP transition pressure is well reproduced, and the experimentally yet inaccessible CP  $\rightarrow$  LP transition pressure is predicted.

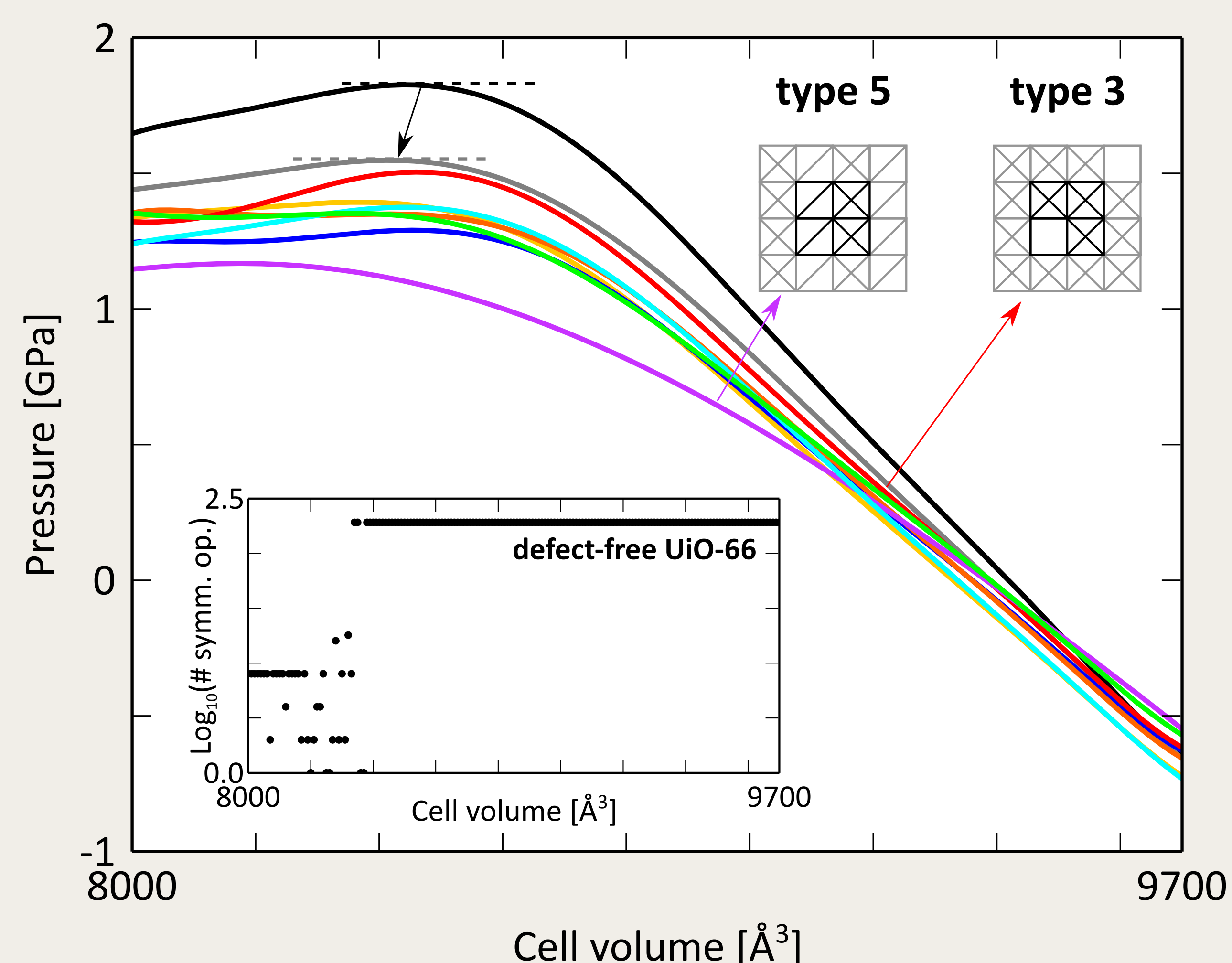
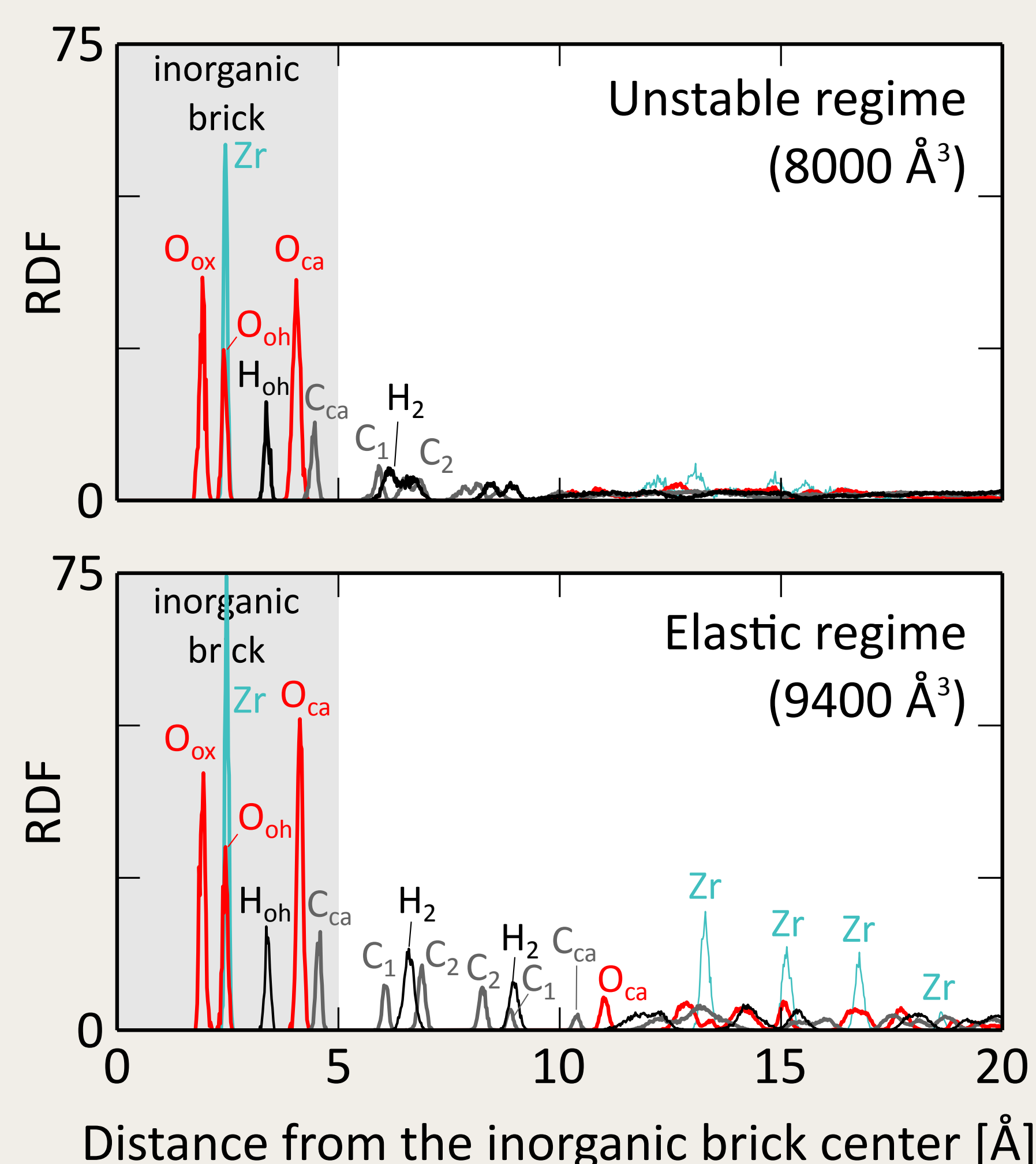


## Pressure-induced loss of crystallinity in UiO-66 depends on the distribution of linker defects [5]

When applying too high a pressure to a UiO-66-type material, the radial distribution function (RDF) reveals a short-range loss of crystallinity

From all 11-fold coordinated UiO-66 materials, the decrease in stability is...

- ... maximum when the removed linkers are oriented in the same direction (**type 5**)
- ... minimum when the removed linkers give rise to a 1D channel (**type 3**)



- 12-fold coordinated**
  - defect-free UiO-66
- 11.5-fold coordinated**
  - type 0
- 11-fold coordinated**
  - type 1
  - type 2
  - type 3
  - type 4
  - type 5
  - type 6
  - type 7



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