Structural Order for One-Scale and Two-Scale Potentials

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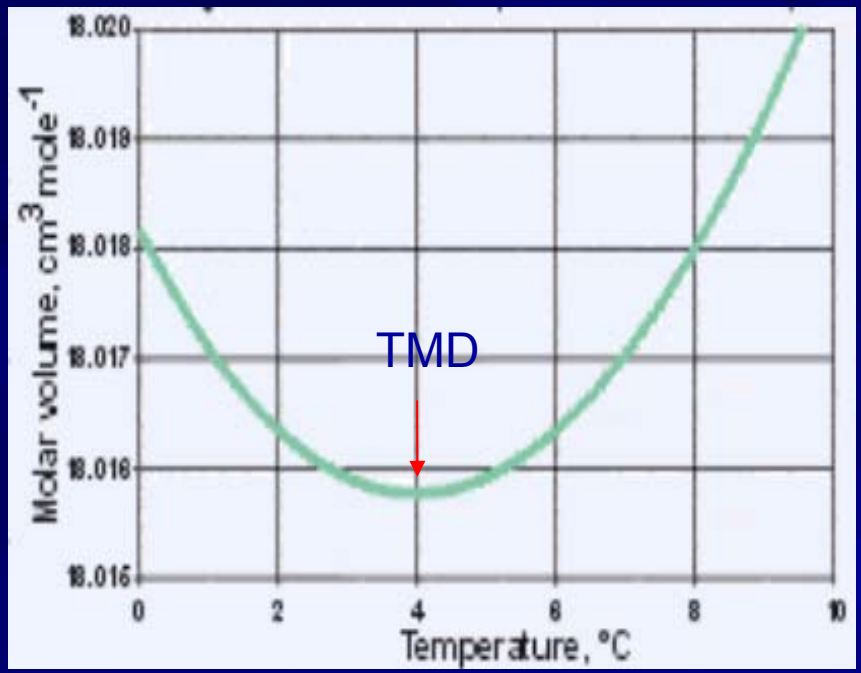
For details see: Phys. Rev. Lett. 95, 130604 (Sep, 2005)

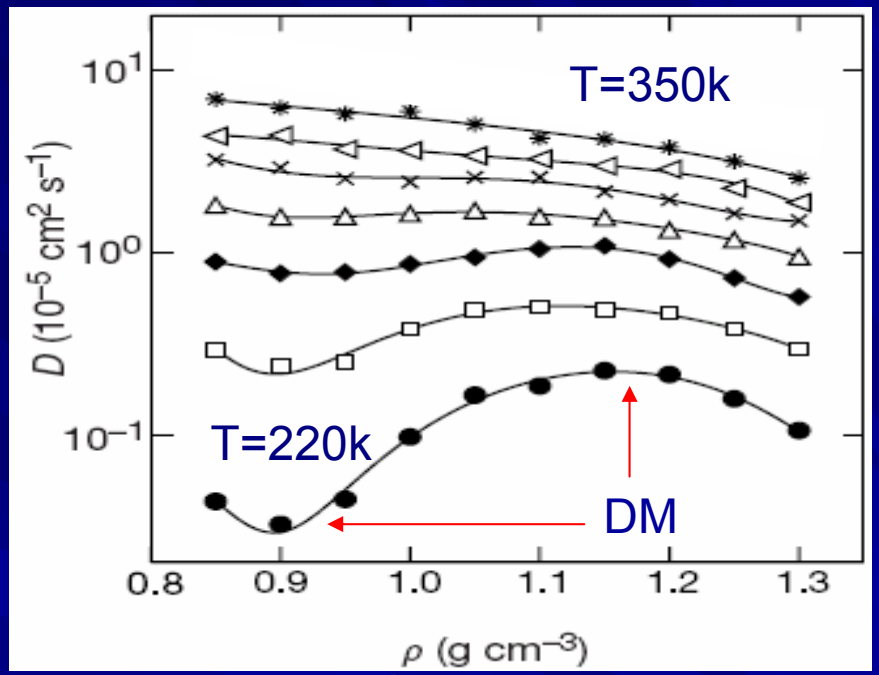
Motivation: anomalies of water

Density anomaly of water



TMD: Temperature of Maximum Density

Diffusion anomaly of water



DM: Diffusion Maximum/Minimum

Recent Finding in water: **structural anomaly coupled with density and diffusion anomaly**

J. R.. Errington and P. G. Debenedetti, Nature 409, 318 (2001).

Questions ?

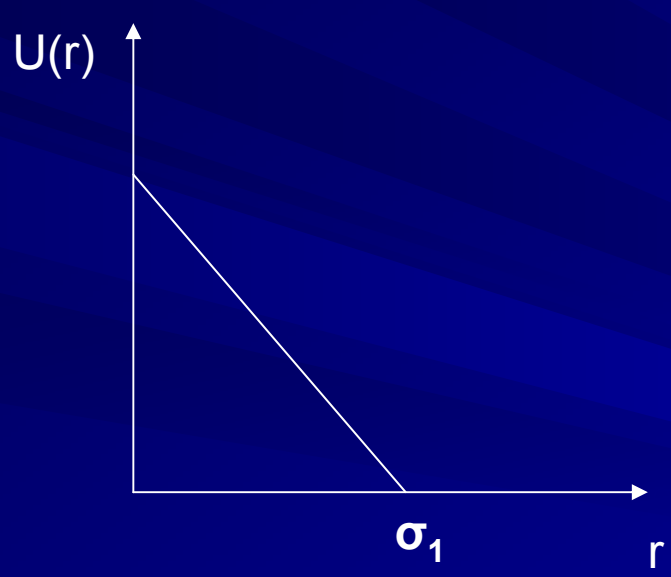
1. Are the strong orientational tetrahedral interactions necessary for water anomalies ?

2. Can we find water-like anomalies in simple liquids (monatomic model with simple potential)?

If YES, then what features should be present in the potential in order to get water-like anomalies ?

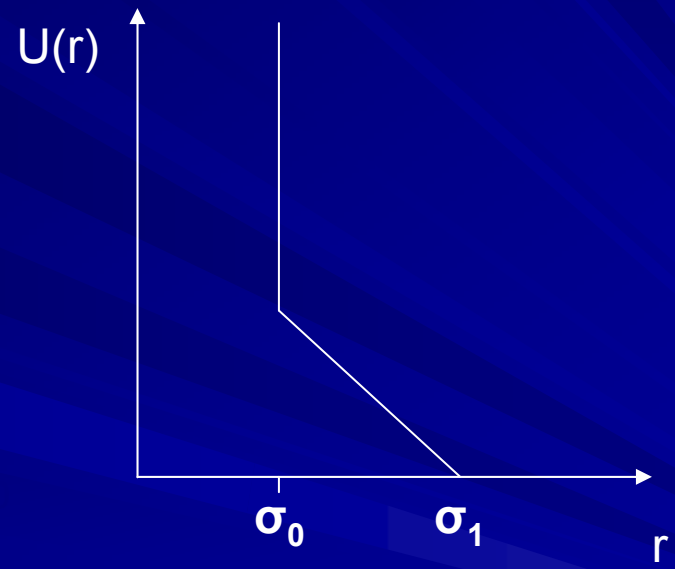
The models: one-scale and two-scale ramp potentials

one-scale



TMD, DM

two-scale



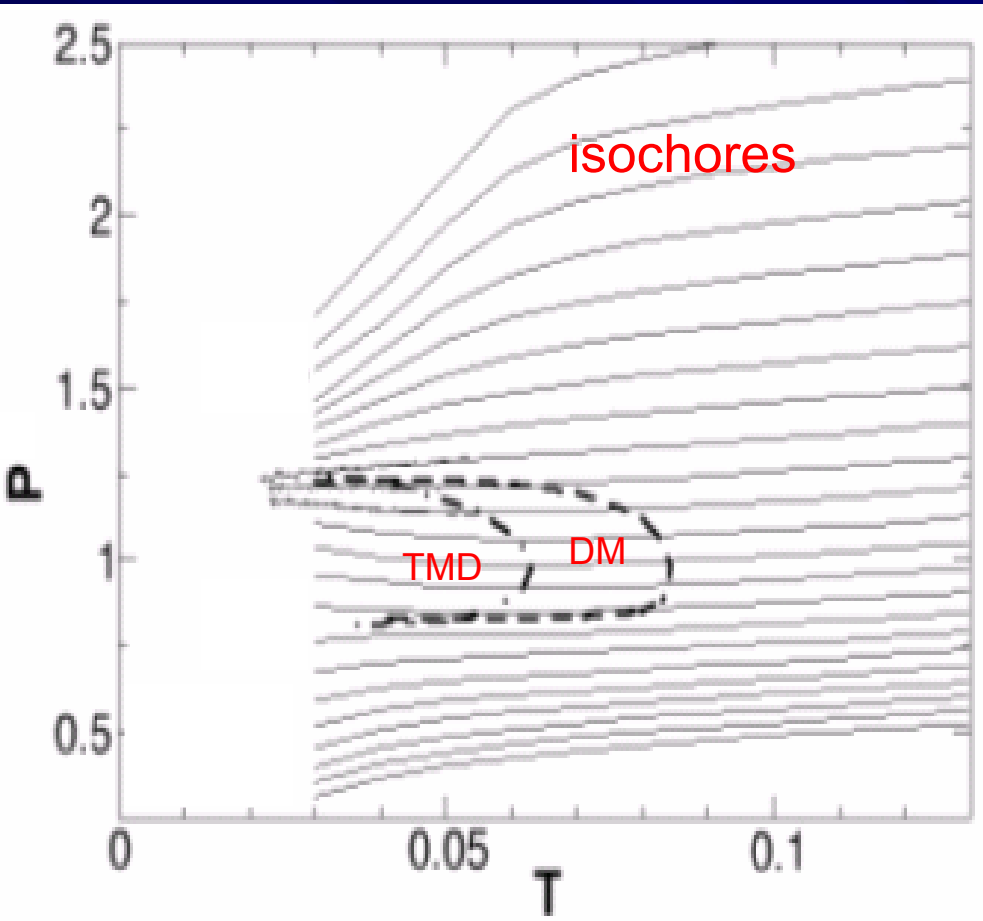
TMD, DM

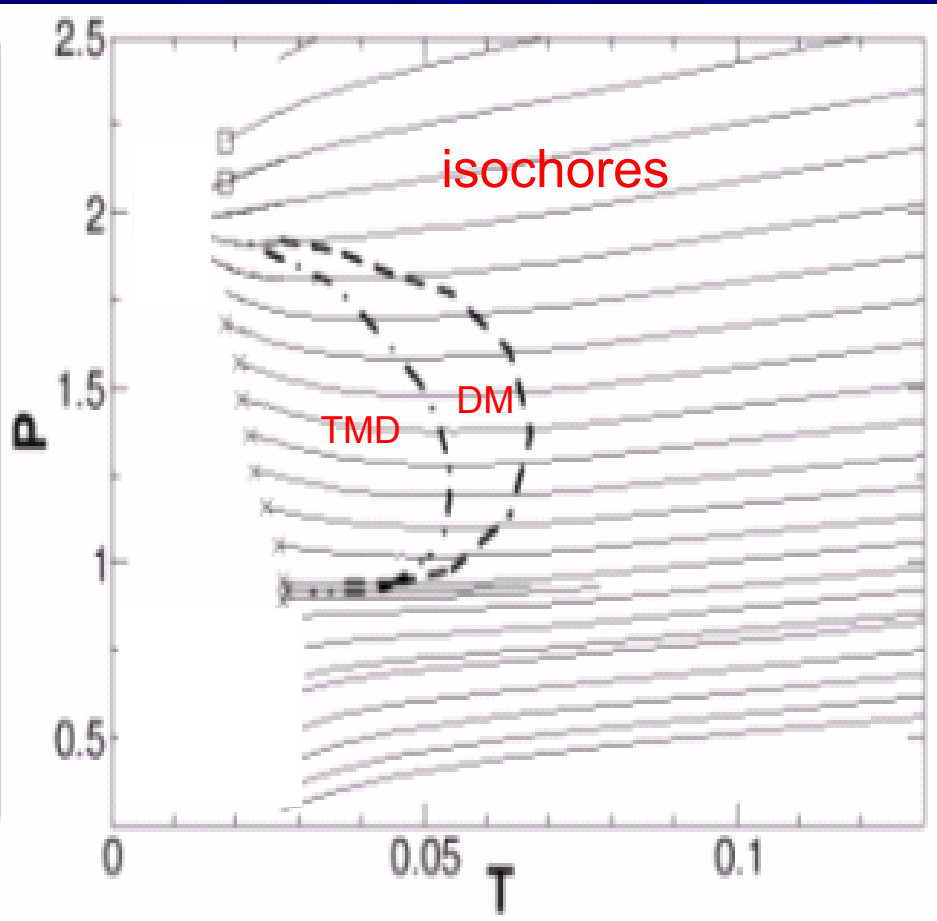
E. A. Jagla, J. Chem. Phys. 111, 8980 (1999)

Result: phase diagrams

One-Scale

Two-Scale





Region of DM encloses the region of TMD

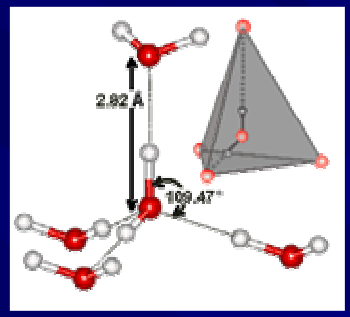
What about the structural anomaly?

How to quantify structural order

Two basic types of order:

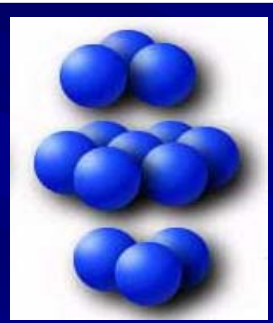
- . Orientational order: degree to adopt specific local structure (space angle)

Water: tetrahedrality,



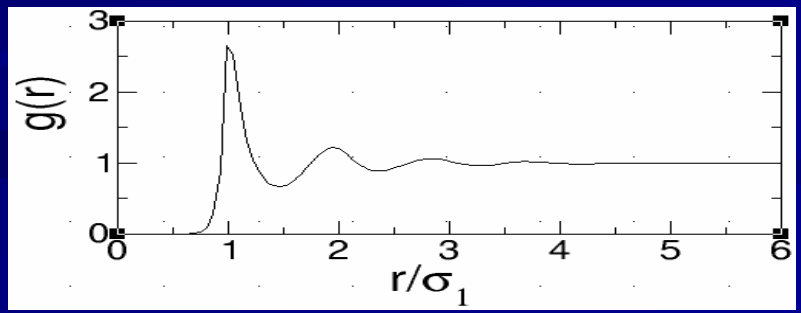
$$q = 1 - \frac{3}{8}\sum_{j=1}^{3}\sum_{k=j+1}^{4}\left(\cos\psi_{jk} + \frac{1}{3}\right)^2$$

Ramp potential: FCC



$$Q_{\ell i} \equiv \left[\frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{m=\ell}|\overline{Y}_{\ell m}|^2\right]^{\frac{1}{2}}$$

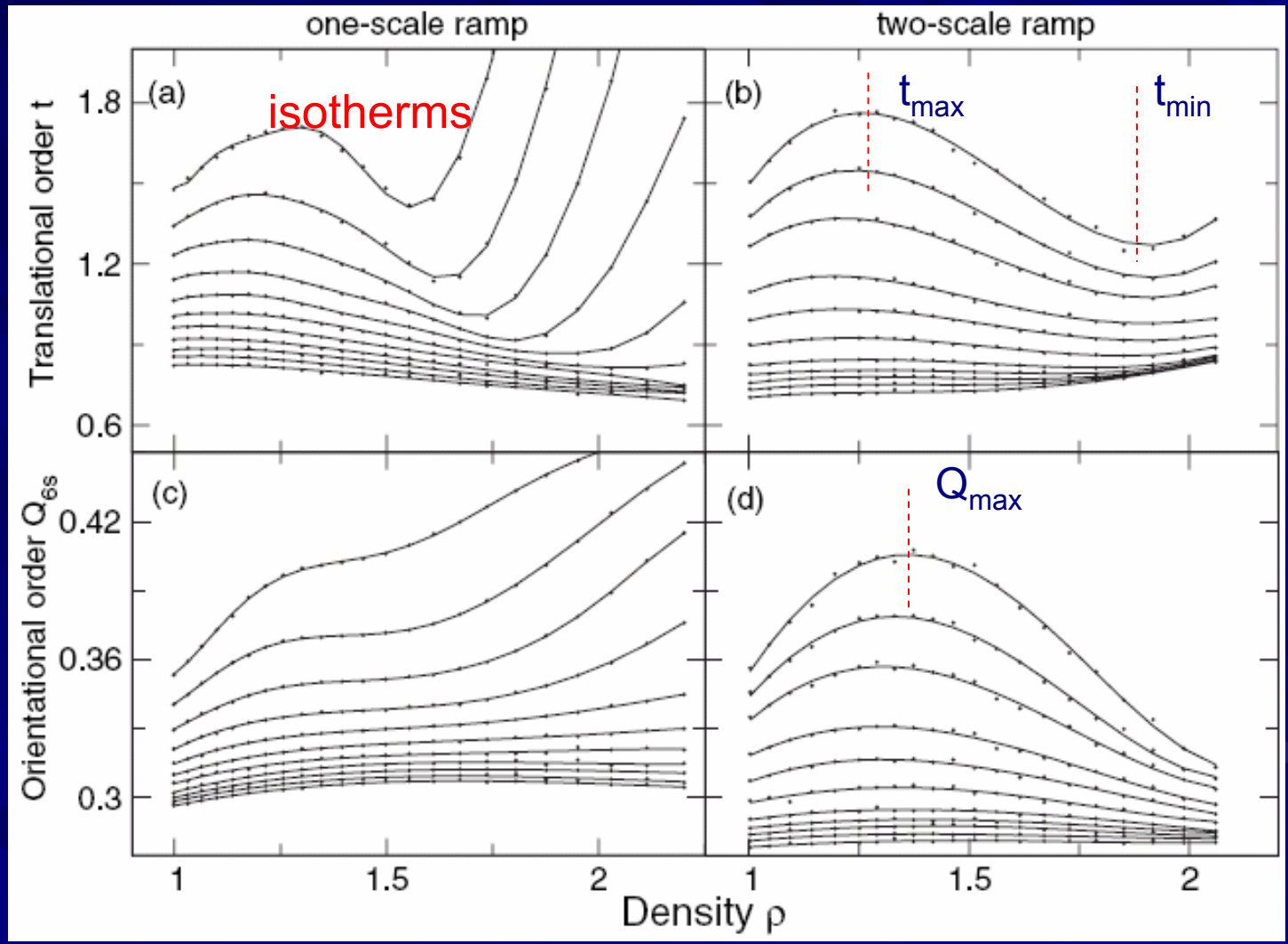
- Translational order t: degree to adopt preferential separations (distance)



$$t \equiv \int_0^{r_c} |g(r) - 1| dr$$

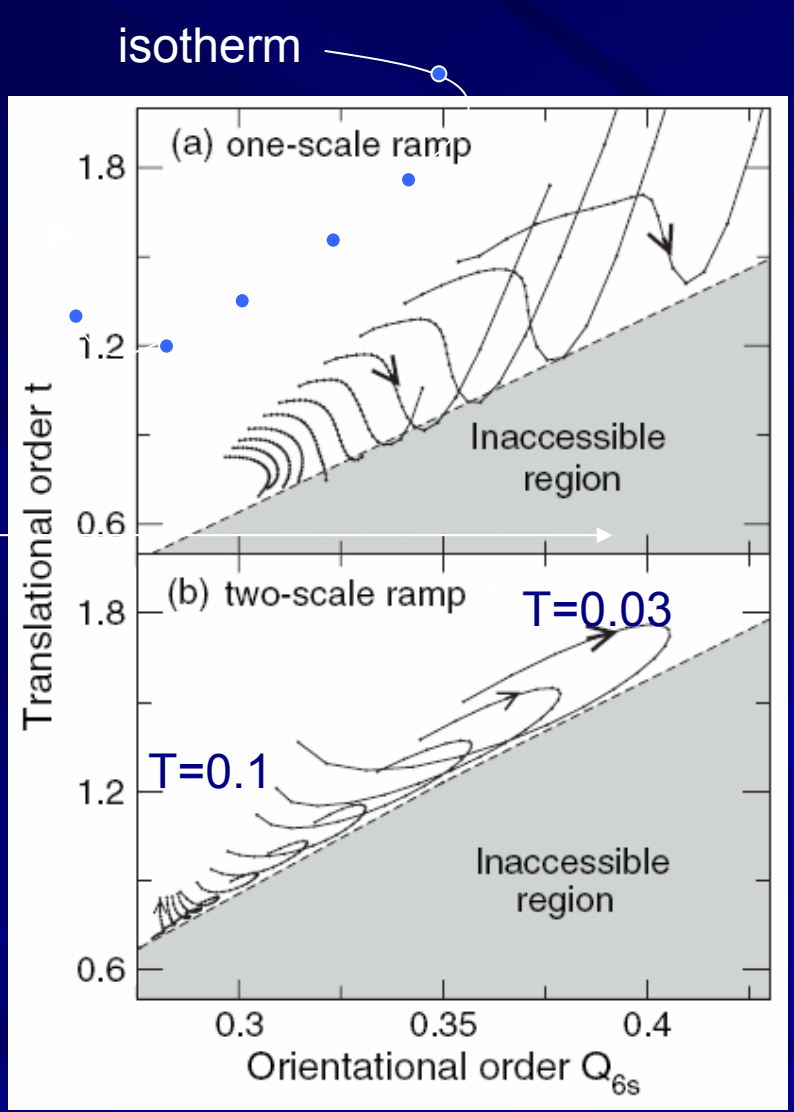
The value increases with increasing order

Result: structural order for ramp potentials

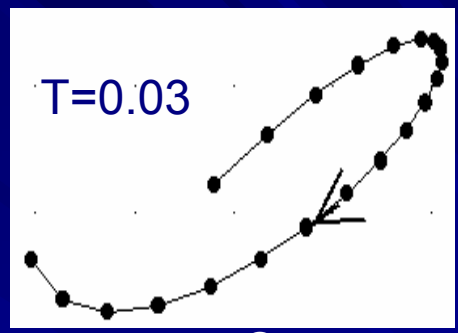


t_{max} and t_{min} for both one-scale and two-scale, Q_{max} only for two-scale ramp

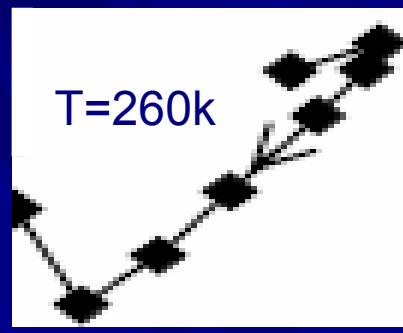
Result: order maps



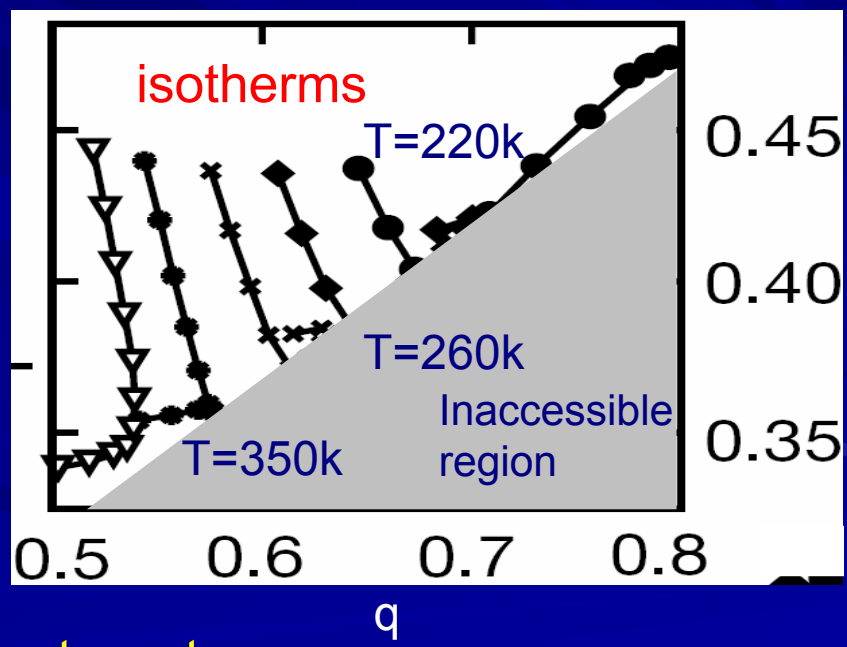
two-scale ramp



water

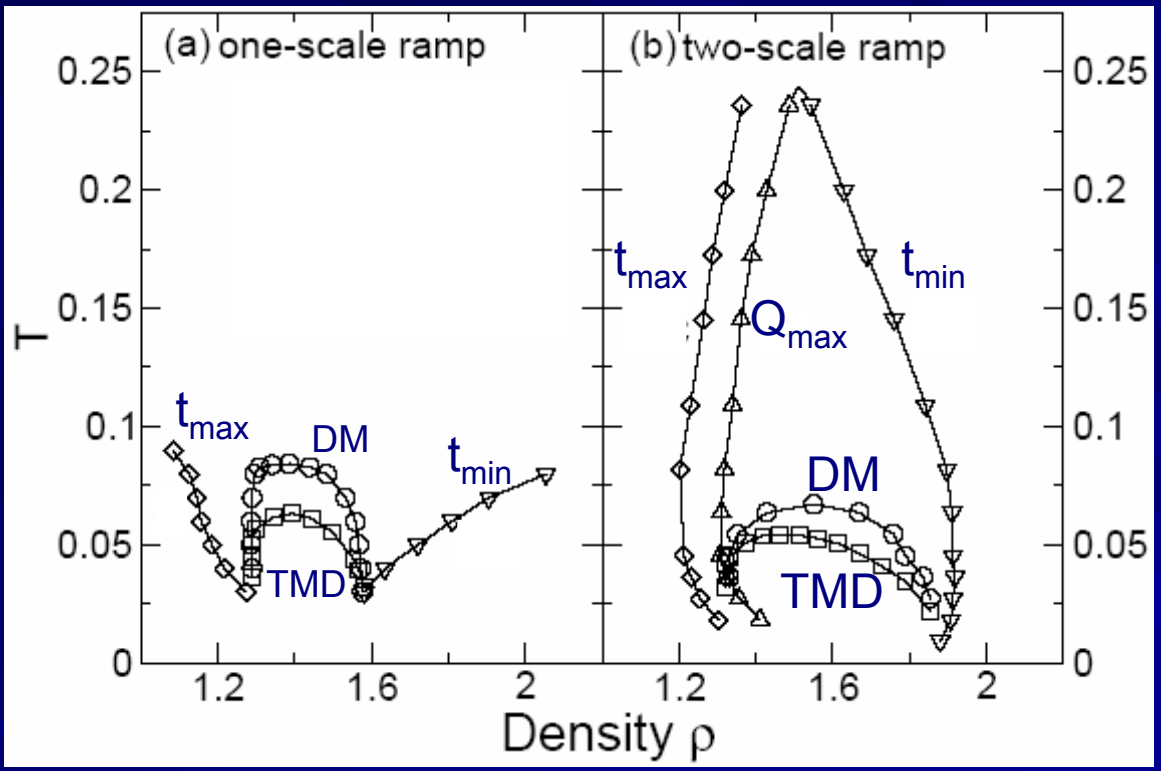


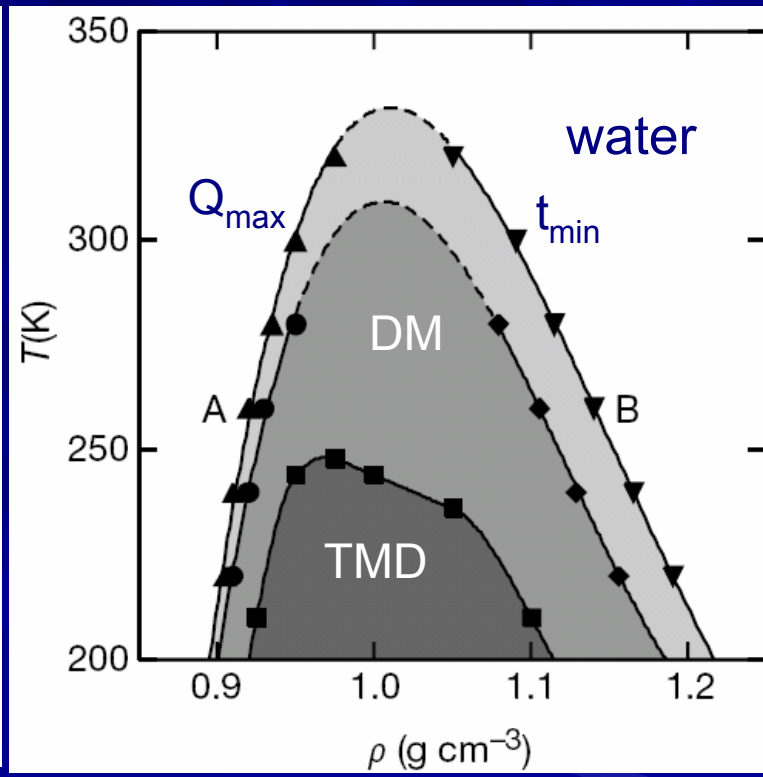
water



Two-scale ramp order map is similar to water

Result: anomalous regions of density, diffusion and structure





Two-scale ramp is similar to water

Summary and Conclusion

1. Are the strong orientational tetrahedral interactions necessary for water anomalies ?

Not necessary

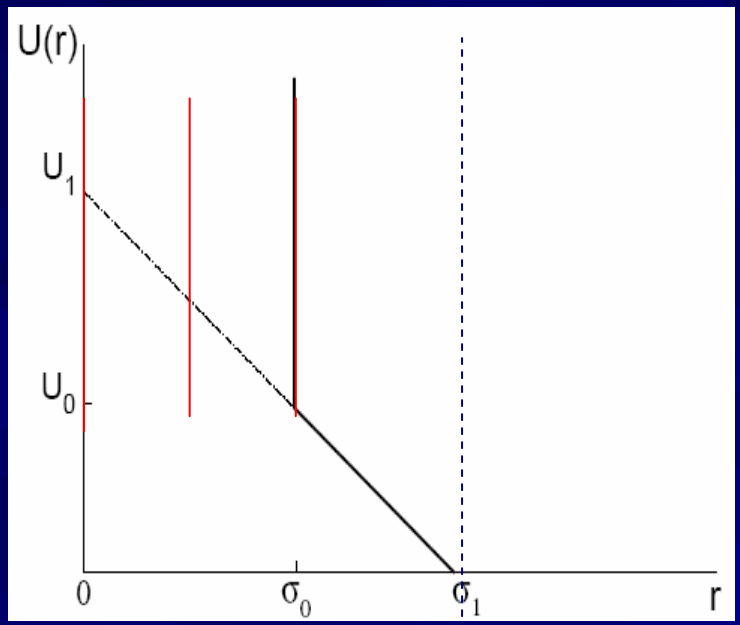
2. Can we find water-like anomalies in simple liquids with simple potentials ?

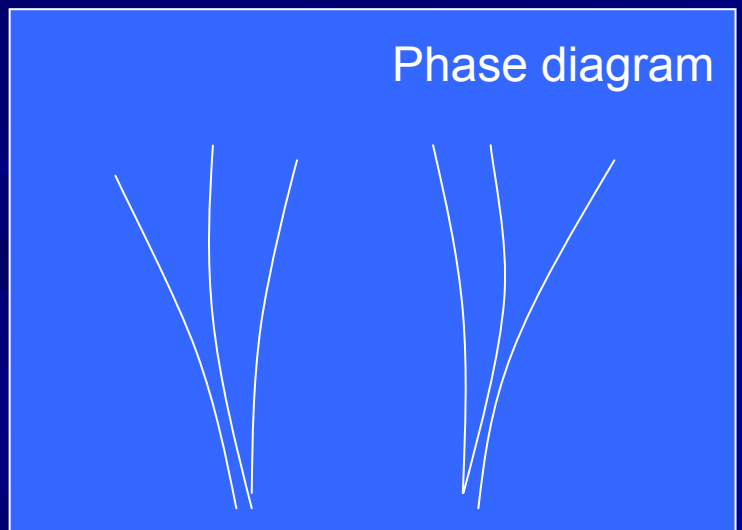
yes

If YES, then what features should be present in the potential in order to get water-like anomalies ?

It suggests that the water-like behavior is related to two characteristic repulsive length scales in potentials.

More





Thank you !