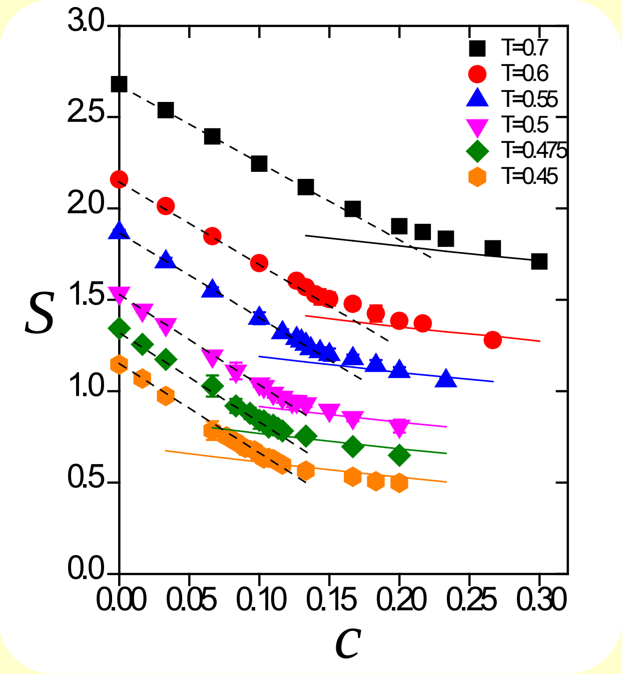
Thermodynamic Glass Transition of Randomly Pinned Systems



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Collaboration

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Kyoto University

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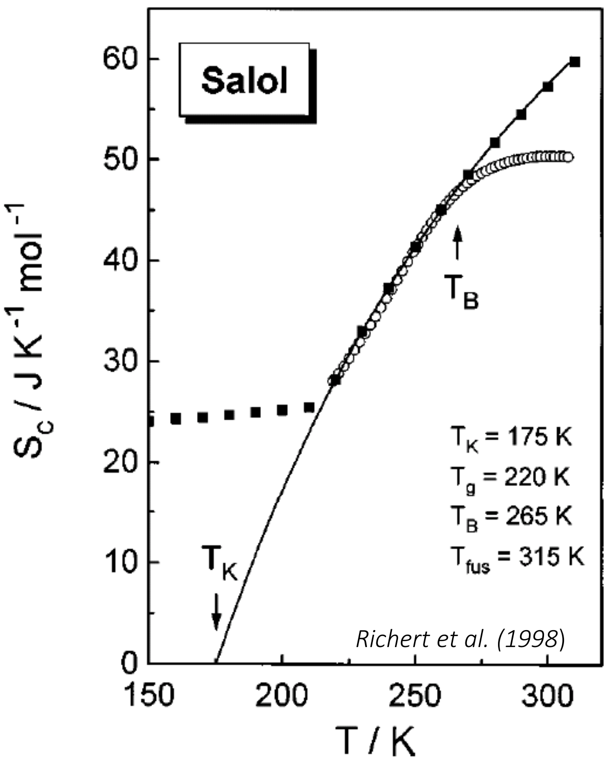
Fluctuation & Structure

科研費
KAKENHI

INTRODUCTION

- Does the *(thermodynamic) Glass Transition Point* exit?

Configuratinal (residual) entropy



Yes!

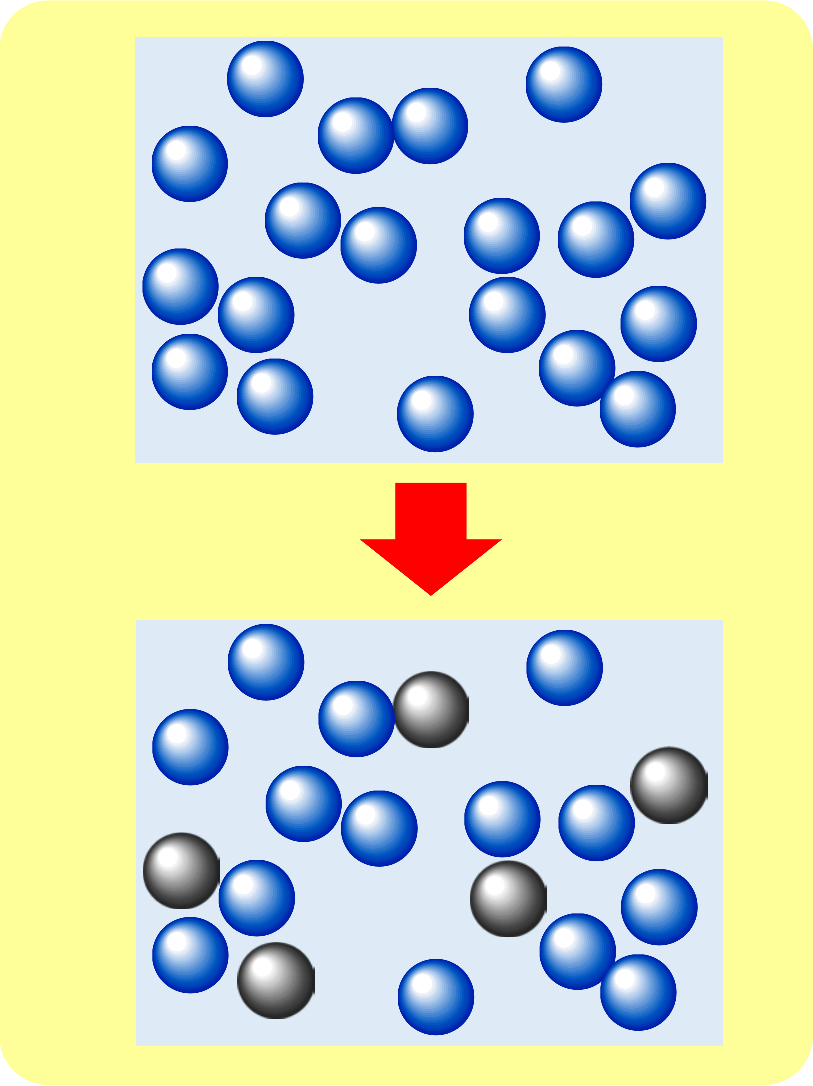
Adam-Gibbs theory
Random First Order Transition(RFOT)
etc…

No!

Purely Kinetic scenarios
Frustration pictures
etc…

RANDOMLY PINNED GLASS

Kim (2000), Krakoviack(2005), KM and others (2009~)



1. Randomly distribute all particles

2. Let them run till equilibrated

3. Quench (pin) a fraction of particles while leave others moving

4. Take ensemble and sample averages

RANDOMLY PINNED GLASS

Cammarota and Biroli (2012)

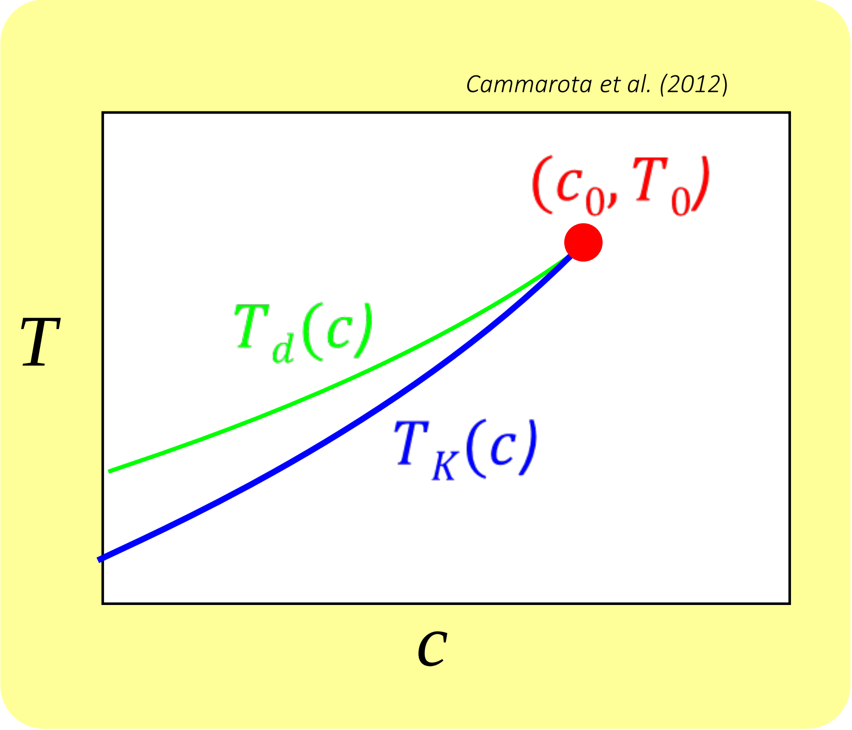
p-spin mean field model with random pinning

$$H = -\sum_{i,j,k} J_{ijk} s_i s_j s_k$$

$$\langle J_{ijk} \rangle = 0, \qquad \langle J_{ijk}^2 \rangle = \frac{3!}{2N^2}$$

- T_K (ideal glass) and T_d (dynamic) transition line rise as c (density of pinned spins) increases.

- They meet and terminate at the end point



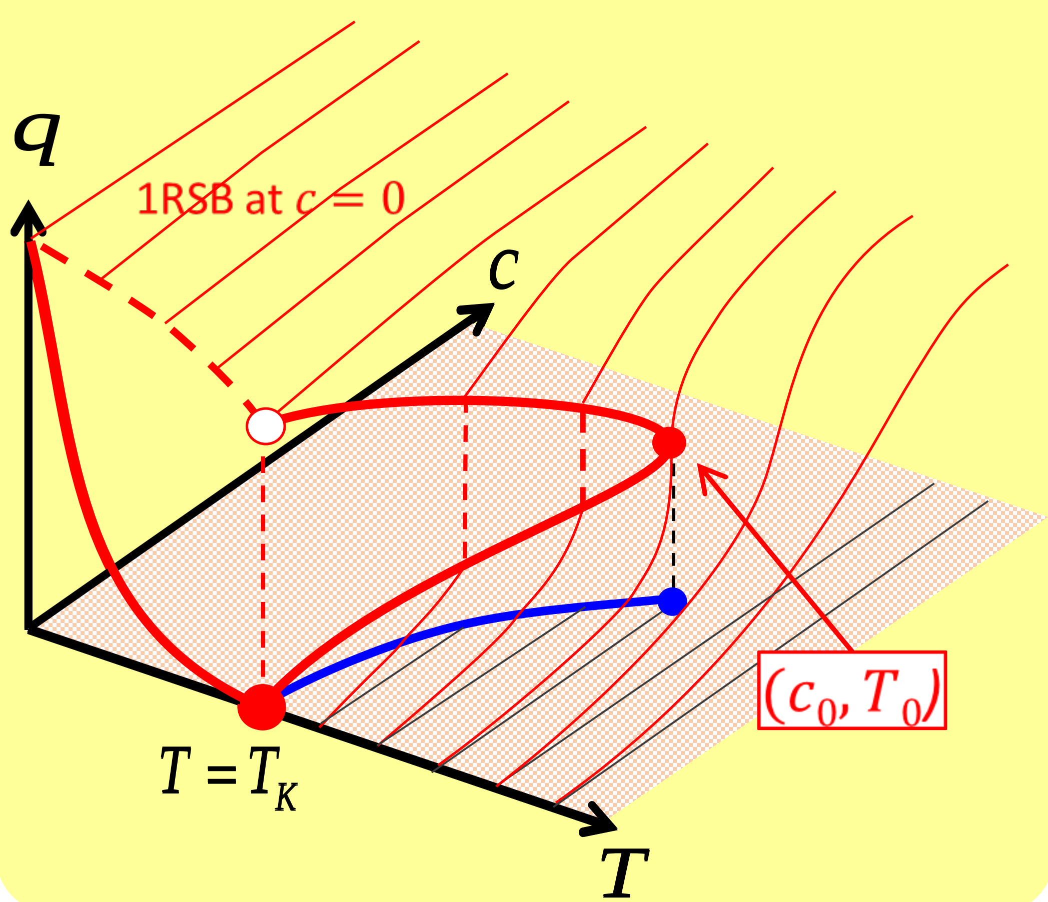
RANDOMLY PINNED GLASS

Cammarota and Biroli (2012)

The ideal glass transition is a mix of 1RSB + 1st order transitions

- The overlap q discontinuously jumps at T_K
- The configurational entropy S_c vanishes at T_K
- The end point (c_0, T_0) is of the universality class of Random Field Ising Model

"The Equation of State of the overlap q"



RANDOMLY PINNED GLASS

Kob and Berthier (2013)

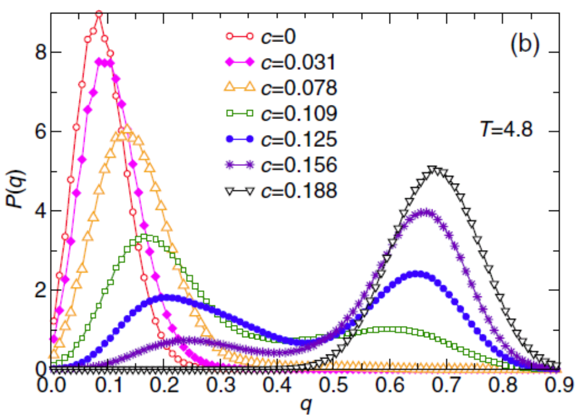
Replica Exchange Simulation for harmonic binary system

Overlap

$$q = \frac{1}{N'}\sum_{i=1}^{N'} n_i^{\alpha} n_i^{\beta}$$

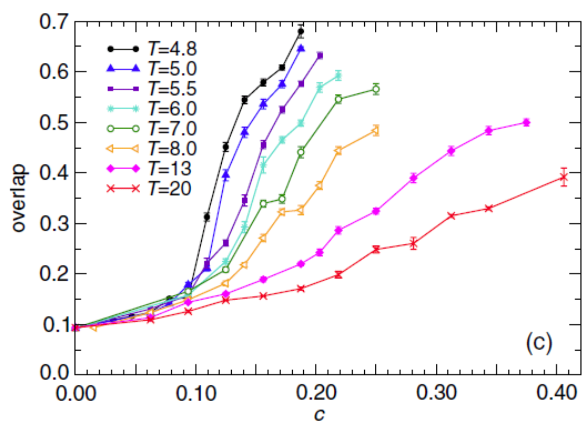
Distribution of q

Double peaked:
The 1st order transition in finite sized box



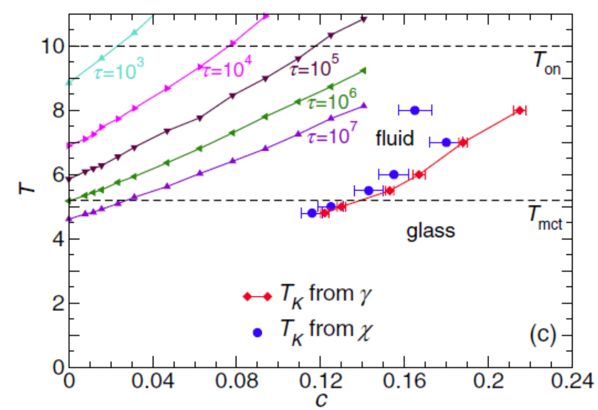
Averaged overlap q

Discontinuous jump



Phase diagram

Ideal glass!



Kob et al. (2013)

RANDOMLY PINNED GLASS

AGENDA

1. Overlap q: discontinuously jump at T_K

2. Configurational Entropy S_c : vanishing at T_K

3. Dynamic Transition (spinodal) line T_d :

   merging with T_K at large c

Model and Simulation Method

System: Kob-Andersen LJ binary mixture

N=300 (and 150)

Simulation methods:

Thermodynamics: Replica Exchange

Dynamics (at higher T): MC

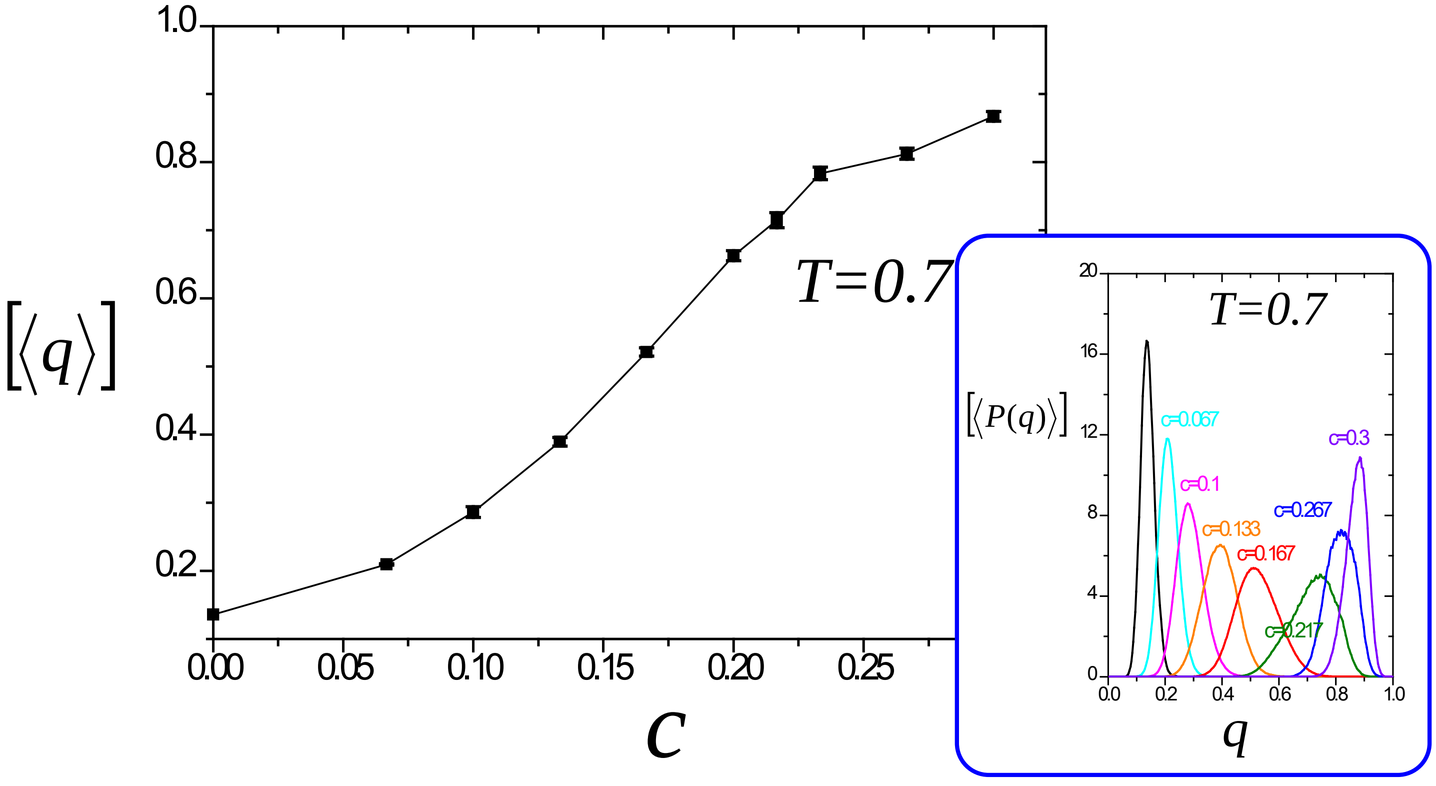
and

Thermodynamic Integration

OVERLAP

Overlap $$q = \frac{1}{N}\sum_{i,j}^{N} \theta(a - |R_i^{\alpha} - R_j^{\beta}|) \qquad (a = 0.3)$$

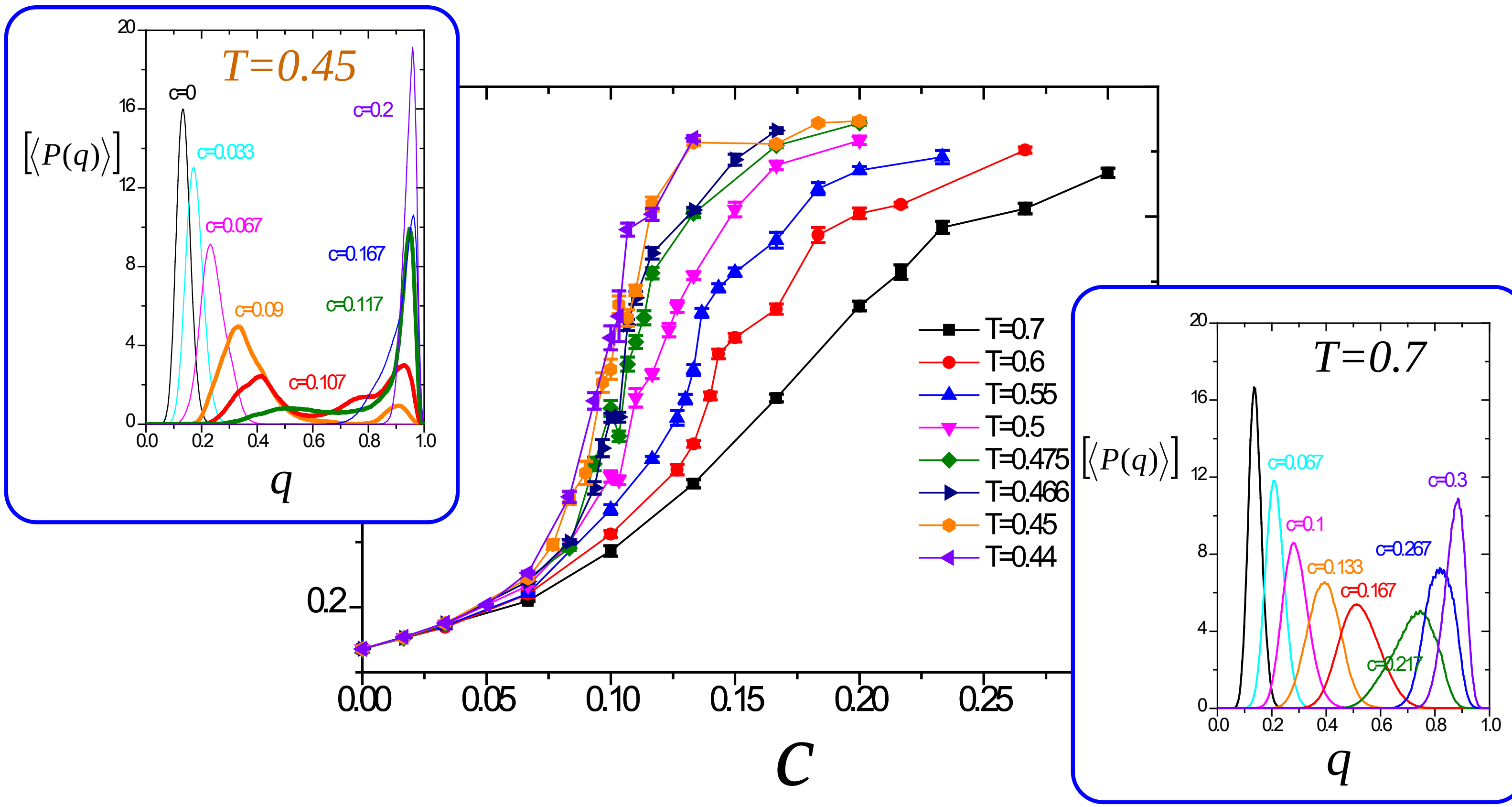
Averaged Overlap



OVERLAP

Overlap $$q = \frac{1}{N}\sum_{i,j}^{N} \theta\left(a - \left|R_i^{\alpha} - R_j^{\beta}\right|\right) \qquad (a = 0.3)$$

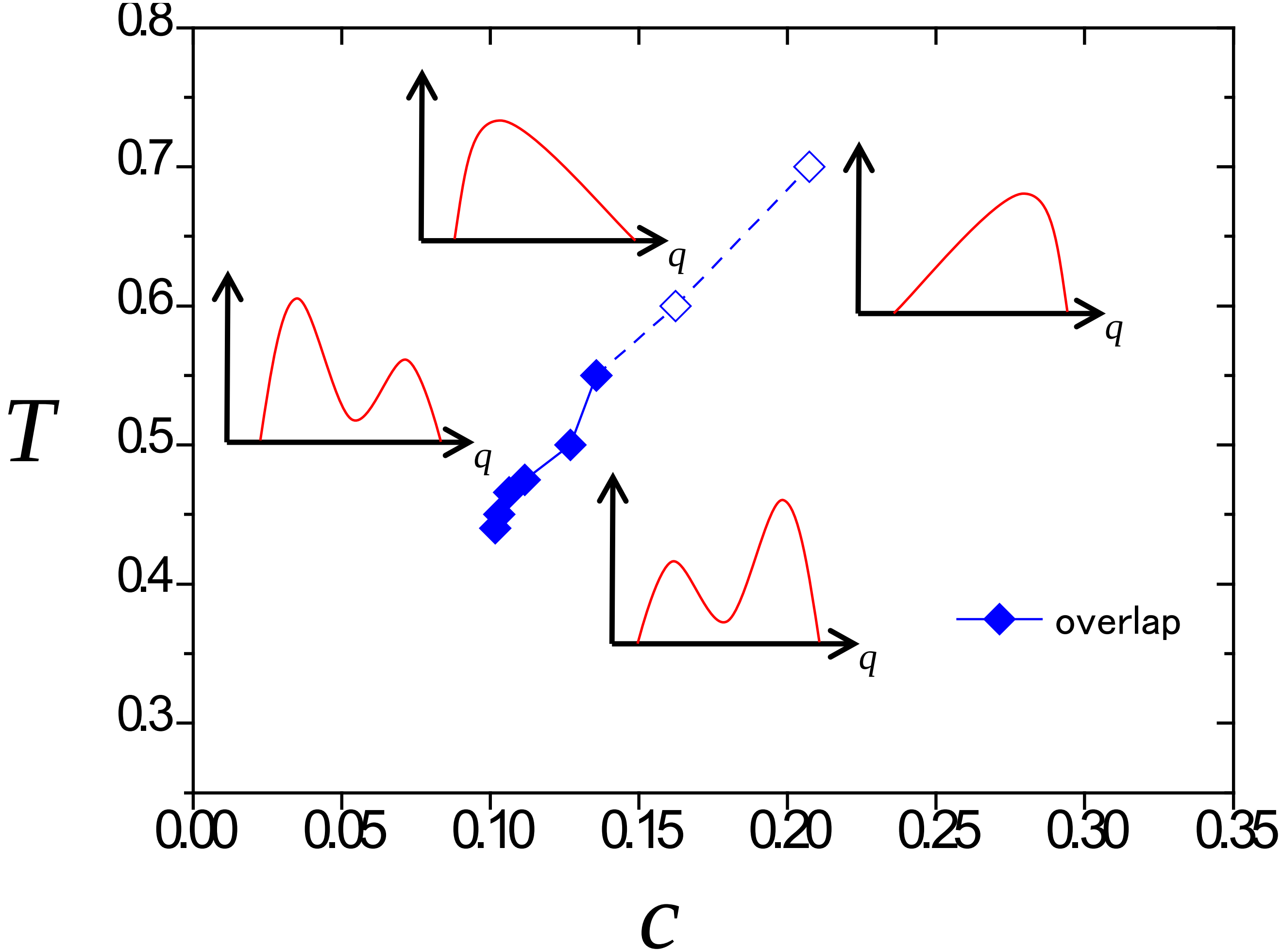
Averaged Overlap



OVERLAP

Phase Diagram

$T_K(c)$ obtained as a point $[\langle P(q) \rangle]$ becomes symmetric



RANDOMLY PINNED GLASS

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CONFIGURATIONAL ENTORPY

Total Entropy of Pinned System

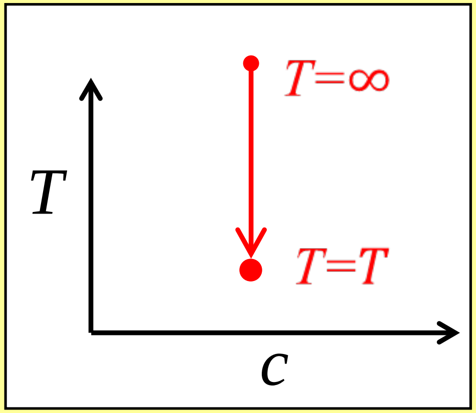
Thermodynamic Integration Method: *Sciortino et al (1999), Coluzzi et al. (2000)*

1. Integrate over a given pinned configuration $\vec{S}$

$$S(\vec{S},\beta) = S(\vec{S},0) + \beta\langle U\rangle(\vec{S},\beta) - \int_0^\beta \mathrm{d}\beta' \ \langle U\rangle(\vec{S},\beta')$$

2. Average over pinned configurations

$$S(\beta) = \left[S(\vec{S},\beta)\right]$$



Vibrational Entropy of Pinned System

1. Harmonic approximation around the inherent structures e_{IS}

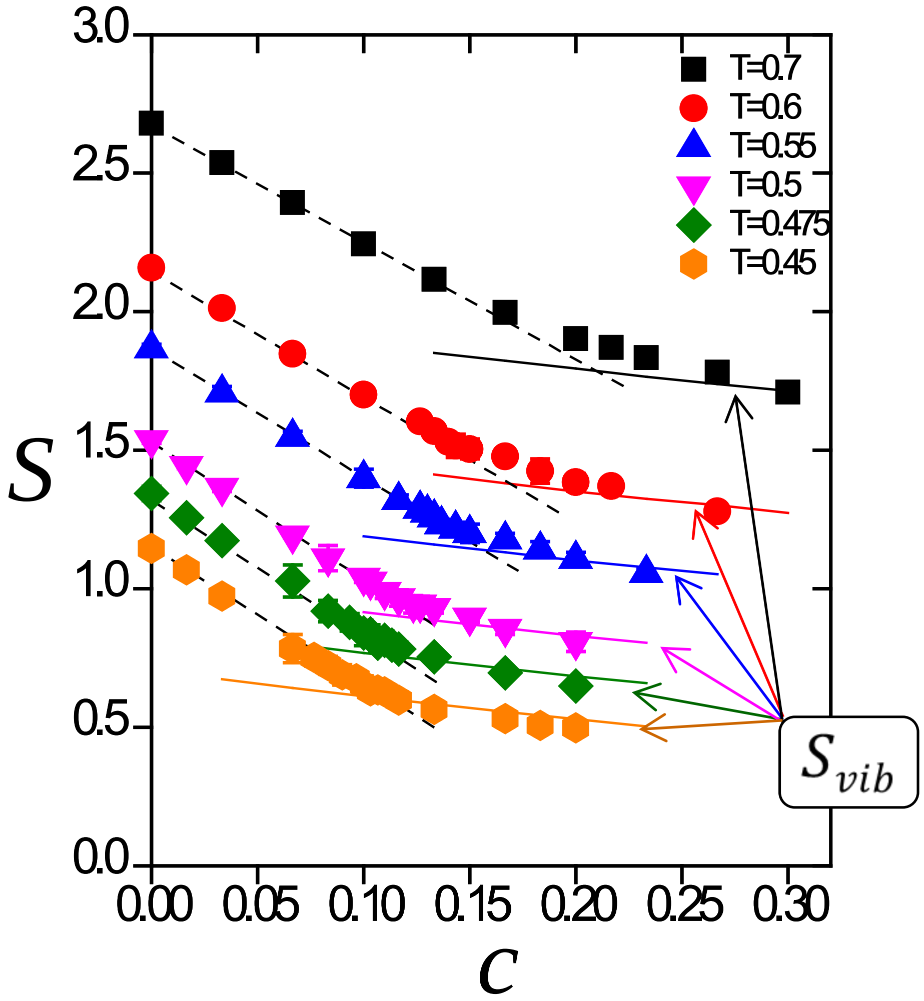
$$S_{\mathrm{vib}}(\vec{S},\beta) = \sum_a \left\{1 - \log\left(\beta\hbar\omega_a\right)\right\}(\vec{S})$$

2. Average over pinned configurations

$$S_{\mathrm{vib}}(\beta) = \left[S_{\mathrm{vib}}(\vec{S},\beta)\right]$$

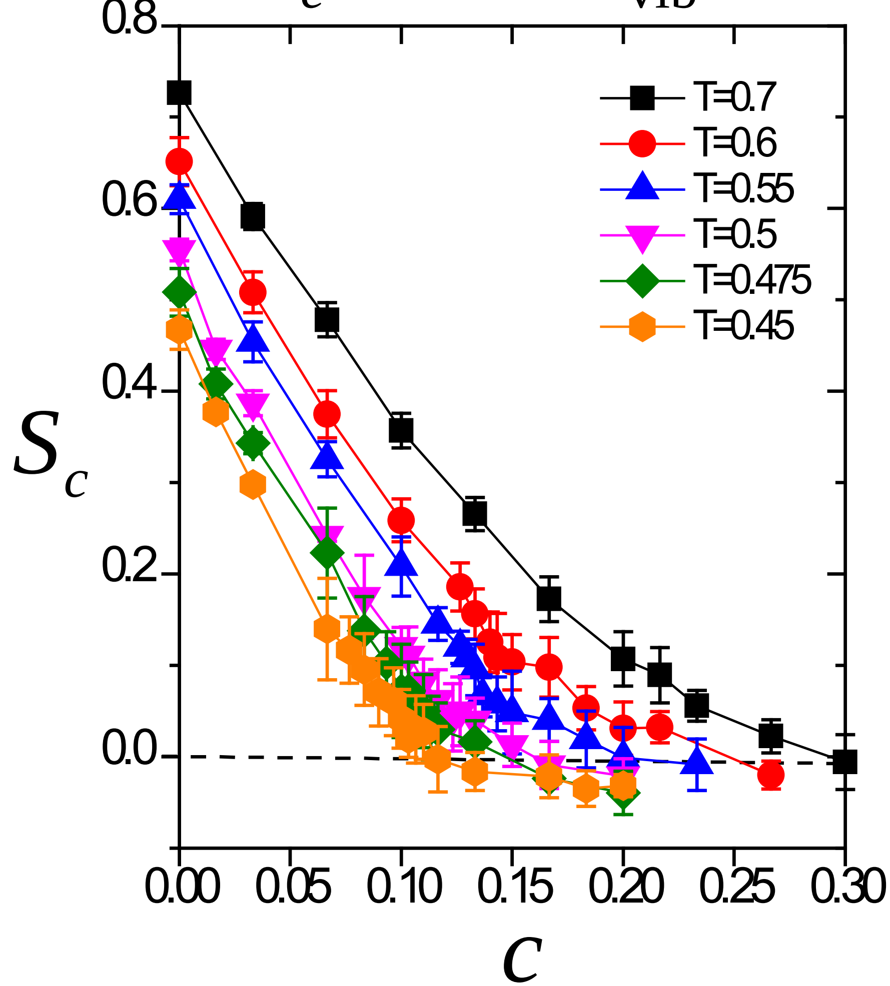
CONFIGURATIONAL ENTORPY

Total Entropy



Configurational Entropy

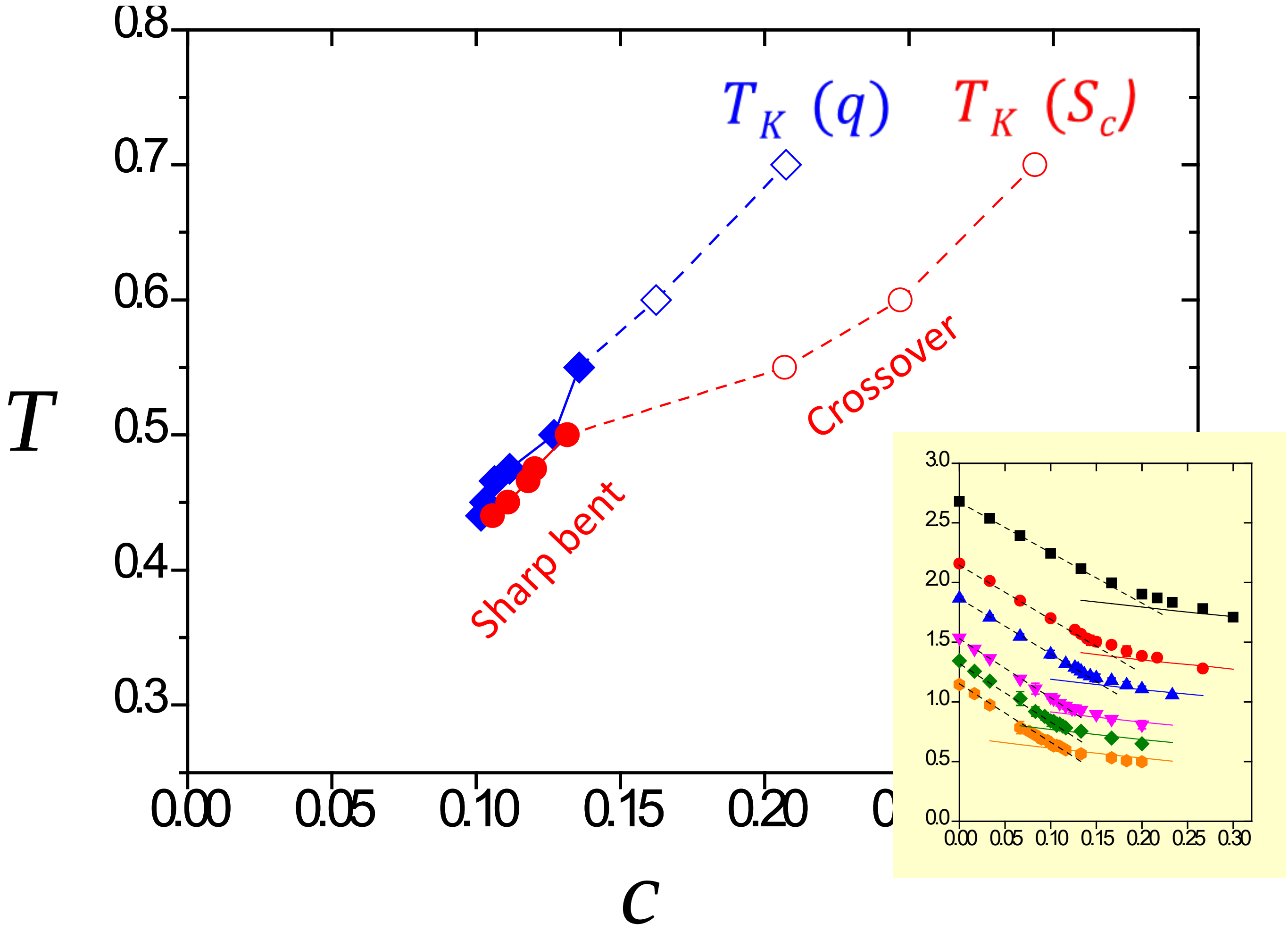
$$S_c = S - S_{\text{vib}}$$



CONFIGURATIONAL ENTORPY

Phase Diagram

$T_K(c)$ obtained as a point where $S_c = 0$



RANDOMLY PINNED GLASS

AGENDA

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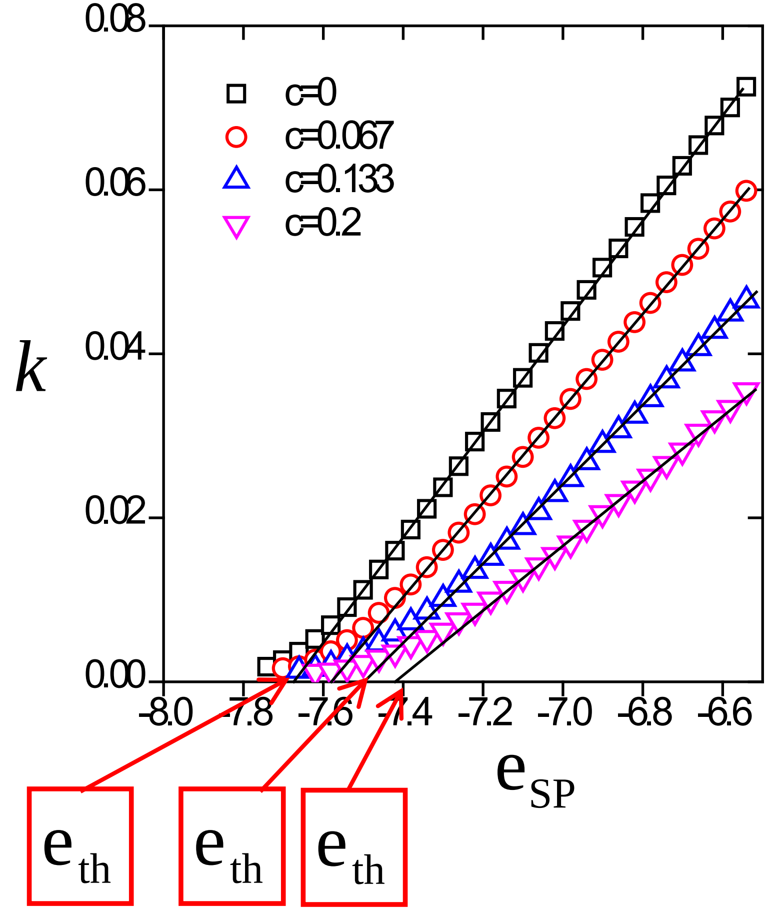
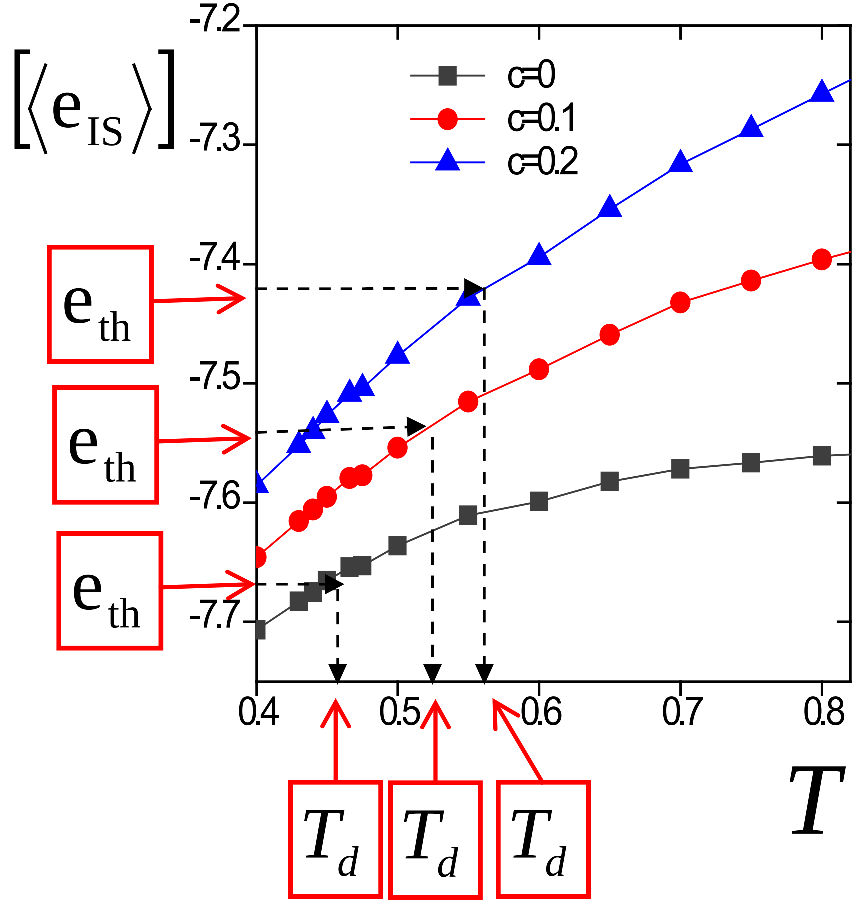
DYNAMIC TRANSITON POINT

The dynamic (MCT) transition T_d (Angelani et al., Broderix et al. 2000)

# of saddles

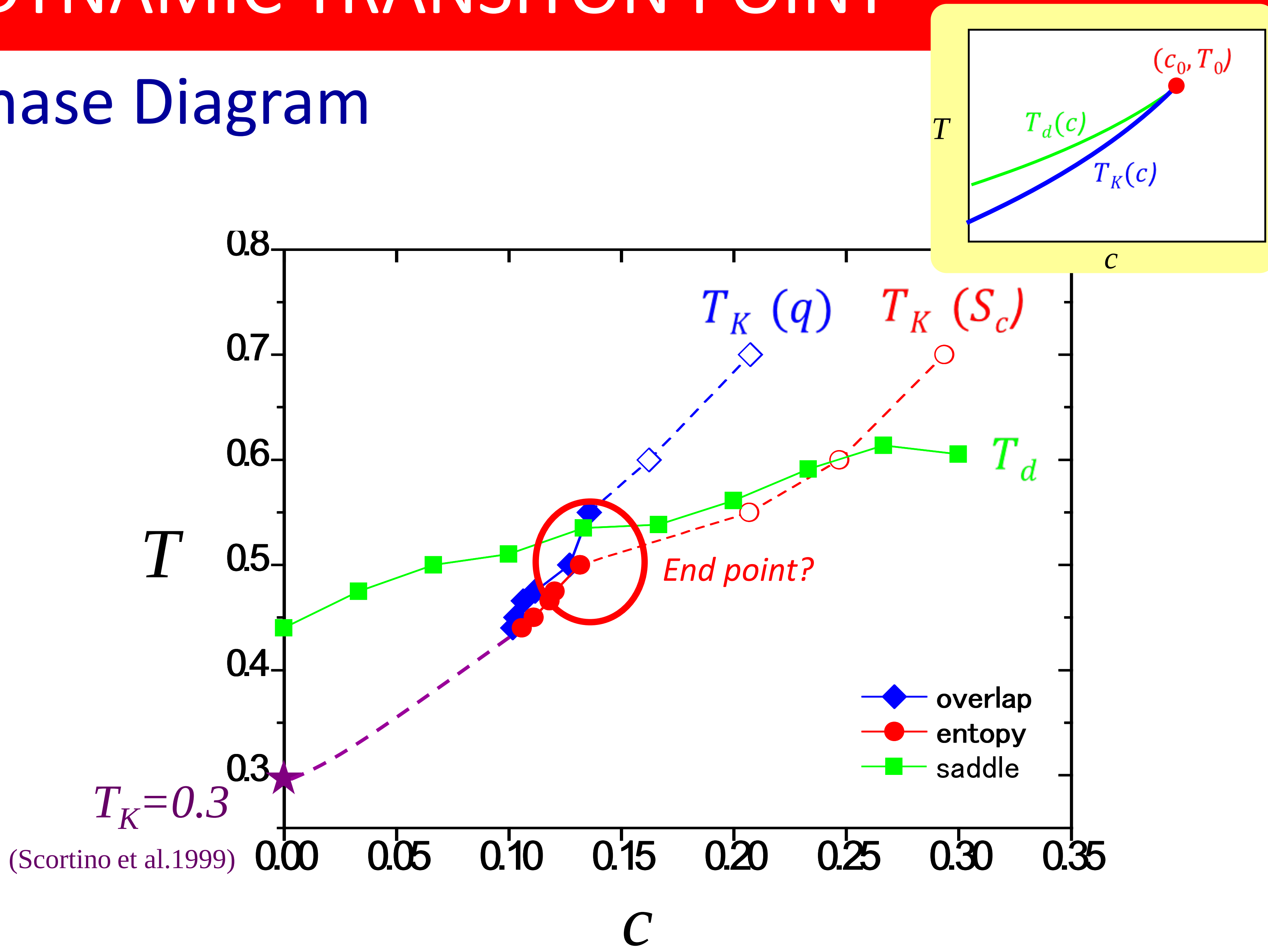


Inherent Structures



DYNAMIC TRANSITON POINT

Phase Diagram



CONCLUSIONS

The first experiments *in silico*
to detect the ideal glass at T_K *and* $Sc = 0$
Strong support for RFOT

More questions than answers

- Glowing *static* length(s) at T_K?
- RFIM universality class at the end point?
- A3 Singular dynamics at the end point?
- and more…