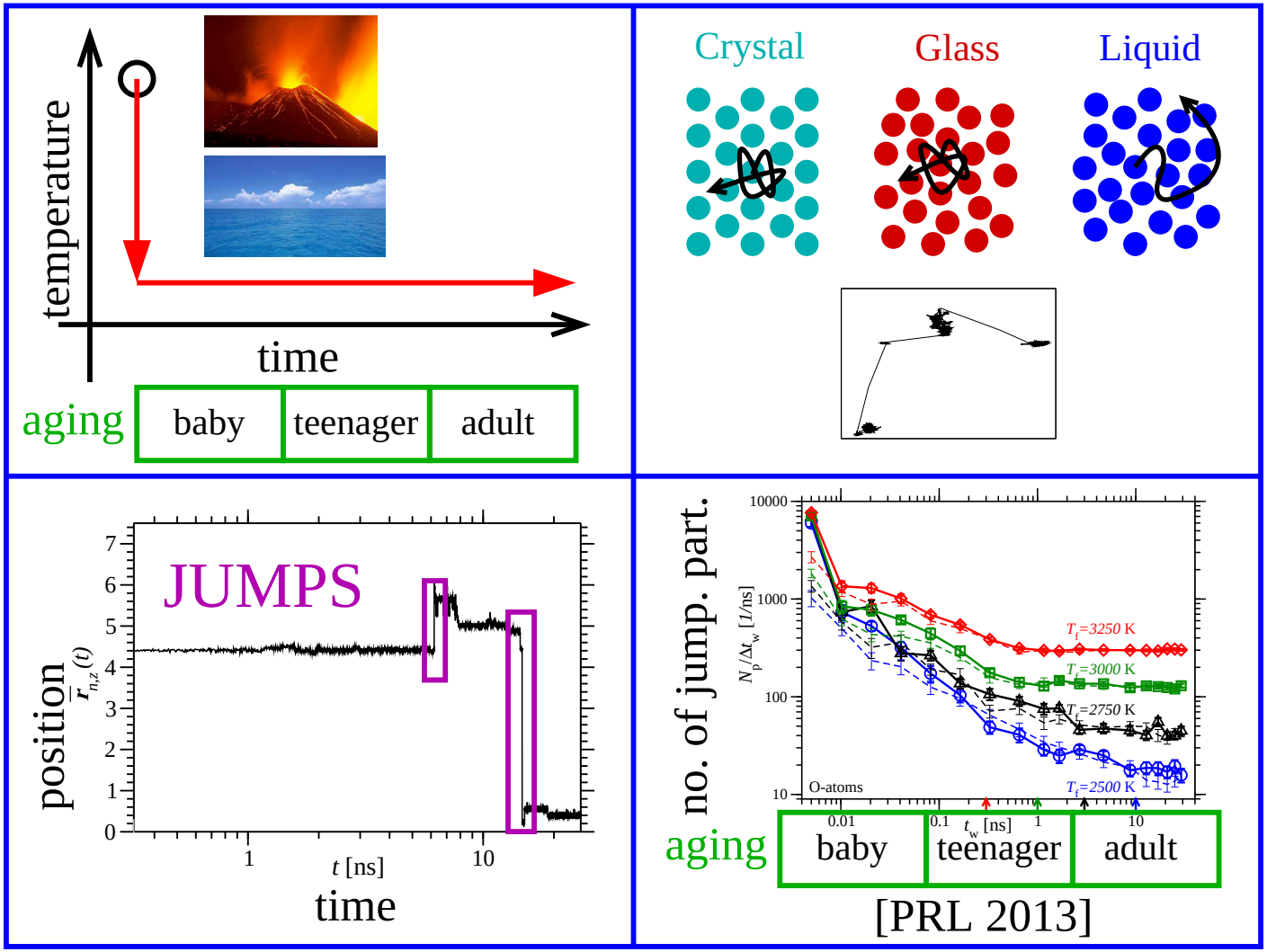
# Katharina Vollmayr-Lee
# Glass Intro & Single Particle Jumps



# Molecular Dynamics Simulation

Initialize:

$\vec{x}_i(t_0),\ \vec{v}_i(t_0),\ \vec{a}_i(t_0)$

particles $i=1,\ldots,N$

three dimensions

$\vec{x}_i(t_0+\Delta t),\ \vec{v}_i(t_0+\Delta t),\ \vec{a}_i(t_0+\Delta t)$

$\vec{x}_i(t_0+2\Delta t),\ \vec{v}_i(t_0+2\Delta t),\ \vec{a}_i(t_0+2\Delta t)$

etc.

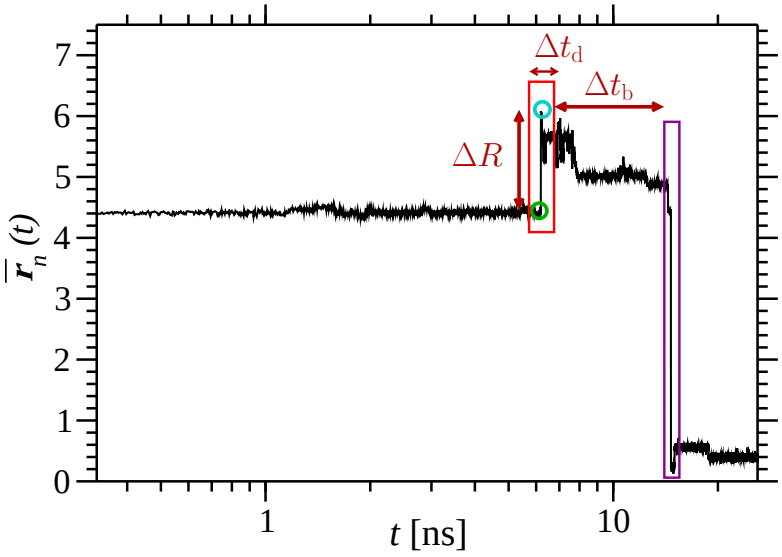
↓ = Iteration Step: (Velocity Verlet)

$$\vec{x}_i(t+\Delta t)=\vec{x}_i(t)+\vec{v}_i(t)\Delta t+\vec{a}_i(t)(\Delta t)^2/2$$

$$\vec{v}_i(t+\Delta t)=\vec{v}_i(t)+(\vec{a}_i(t)+\vec{a}_i(t+\Delta t))\,\Delta t/2$$

$$\vec{a}_i(t)=\vec{F}_i(t)/m_i = -\vec{\nabla}_i U(t)/m_i$$

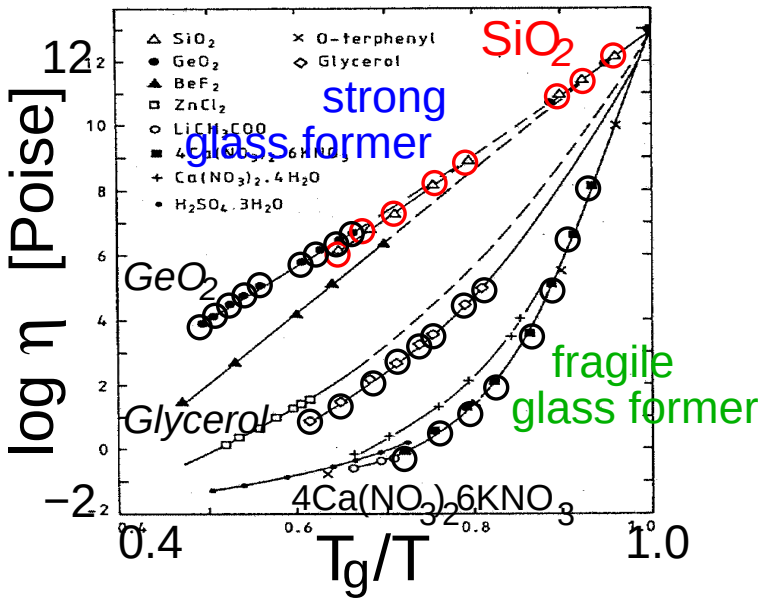
# Summary of $SiO_2$ Results




## Single Particle Jump Dynamics:

- Jump-Size and Time in Cage $t_w$-independent!
- Number of Jumping Particles $t_w$-dependent

[KVL, R. Bjorkquist, L. Chambers, PRL 2013]



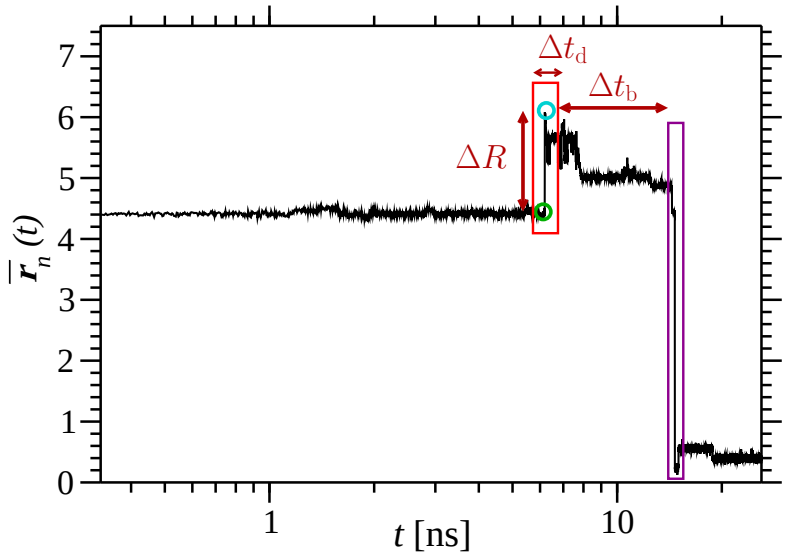

[C.A. Angell and W. Sichina, Ann. NY Acad. Sci. 279, 53

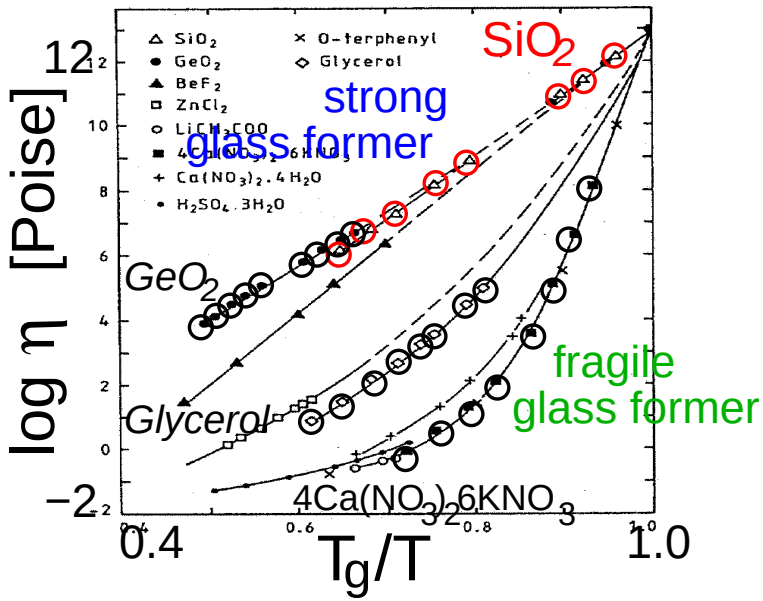
## Comparison:

compare with fragile glass former [Warren, Rottler],[Helfferich et al.]

Surprising similarity
of strong and fragile glass formers

# Newest $SiO_2$ Results




## Clusters of Jumping Particles

- Cluster size distribution exponetial ($SiO_2$; 100000 particles) (summer 2014 REU: Jonathan Cookmeyer; [APS March 2015])
- Cluster size distribution power law (binary LJ; 1000 particles) ([KVL & E. A. Baker, EPL 76, 1130 (2006)])

$\longrightarrow$ Cluster Size Analysis for 100000 binary LJ