Keller group
Theoretical Chemistry: Molecular Dynamics

Research & Drinks
Freie Universität Berlin

Bettina Keller
Freie Universität Berlin

Molecular dynamics

Electronic energy

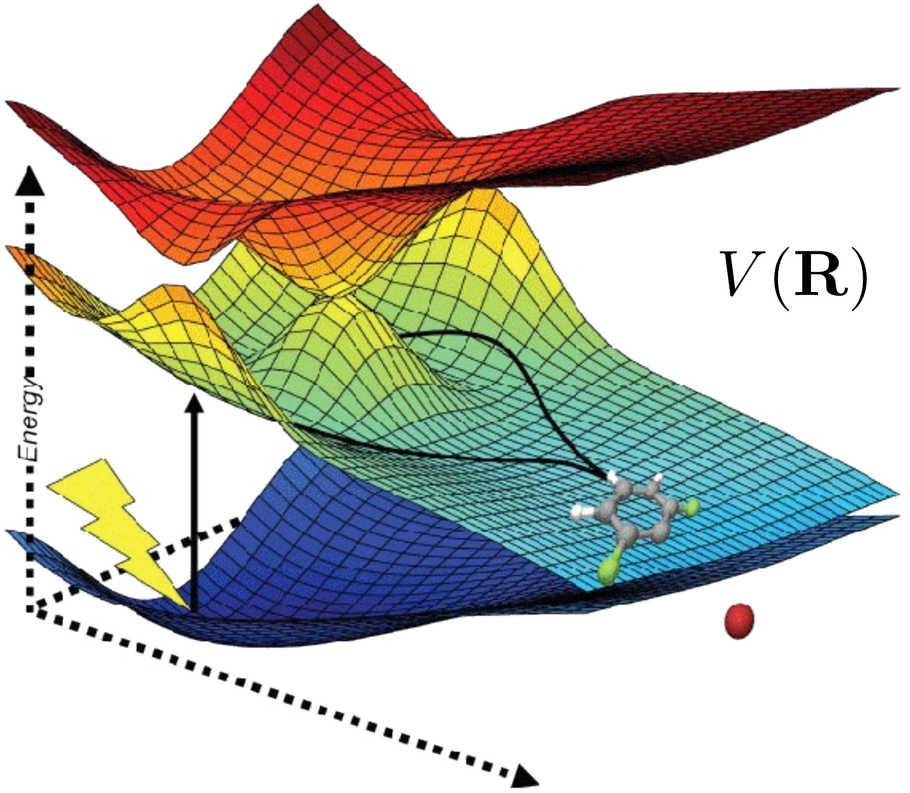
$$\hat{H}_{\mathrm{el}}\psi_k = E_{\mathrm{el}}\psi_k$$

$$V(\mathbf{R}) = V_{NN}(\mathbf{R}) + E_{\mathrm{el}}(\mathbf{R})$$

Various approximations

- DFT
- Neural-Network-Potentials
- Empirical Force Fields

Born-Oppenheimer surface



$V(\mathbf{R})$

Classical dynamics

$$\mathbf{F}_i(t) = -\nabla_i V(\mathbf{R}(t))$$

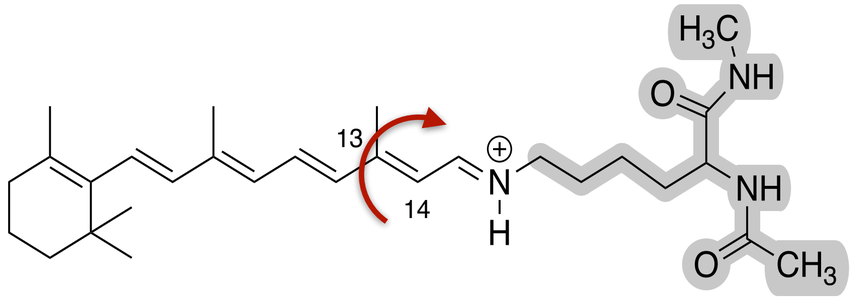
computer simulations

Molecular trajectories

$$\mathbf{R}(t)$$

Simulating chemical reactions

thermal cis-trans isomerization in retinal



10^{19}

simulation timestep

10^{-15} 10^{-14} 10^{-13} 10^{-12} 10^{-11} 10^{-10} 10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} s

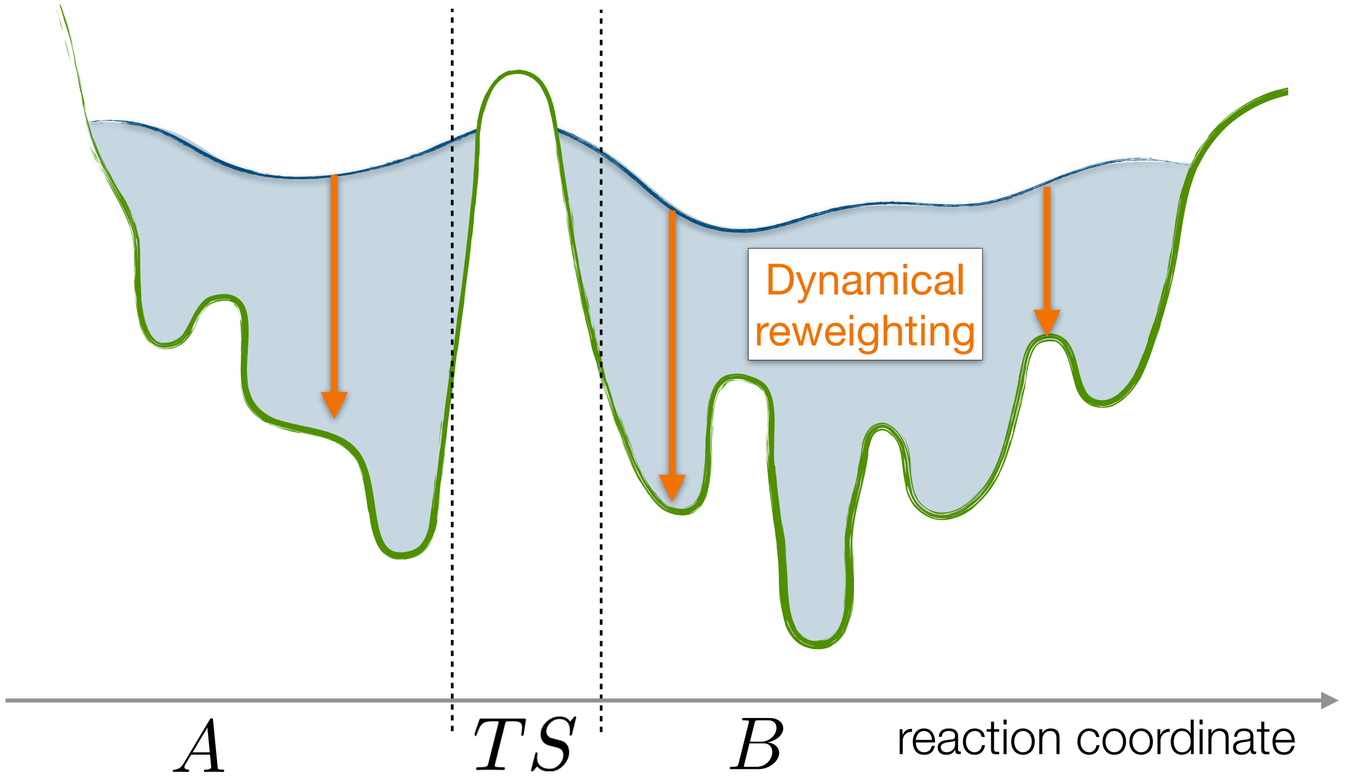
timescale of the reaction

movie frame rate

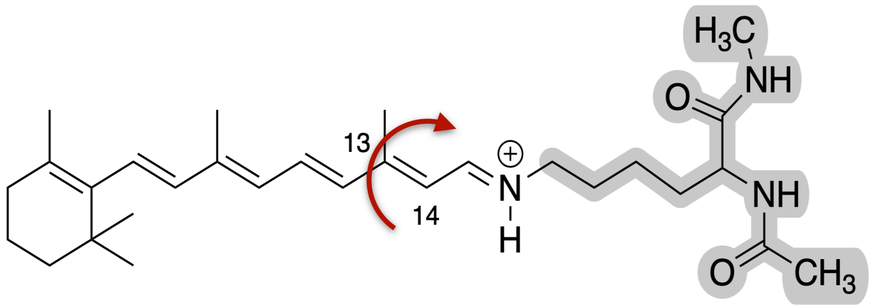
10^{-2} 10^{-1} 10^{0} 10^{2} 10^{3} 10^{4} 10^{5} 10^{6} 10^{7} 10^{8} 10^{9} 10^{10} 10^{11} 10^{12} 10^{13} 10^{14} 10^{15} 10^{16} 10^{17} s

age of the universe

Simulating chemical reactions

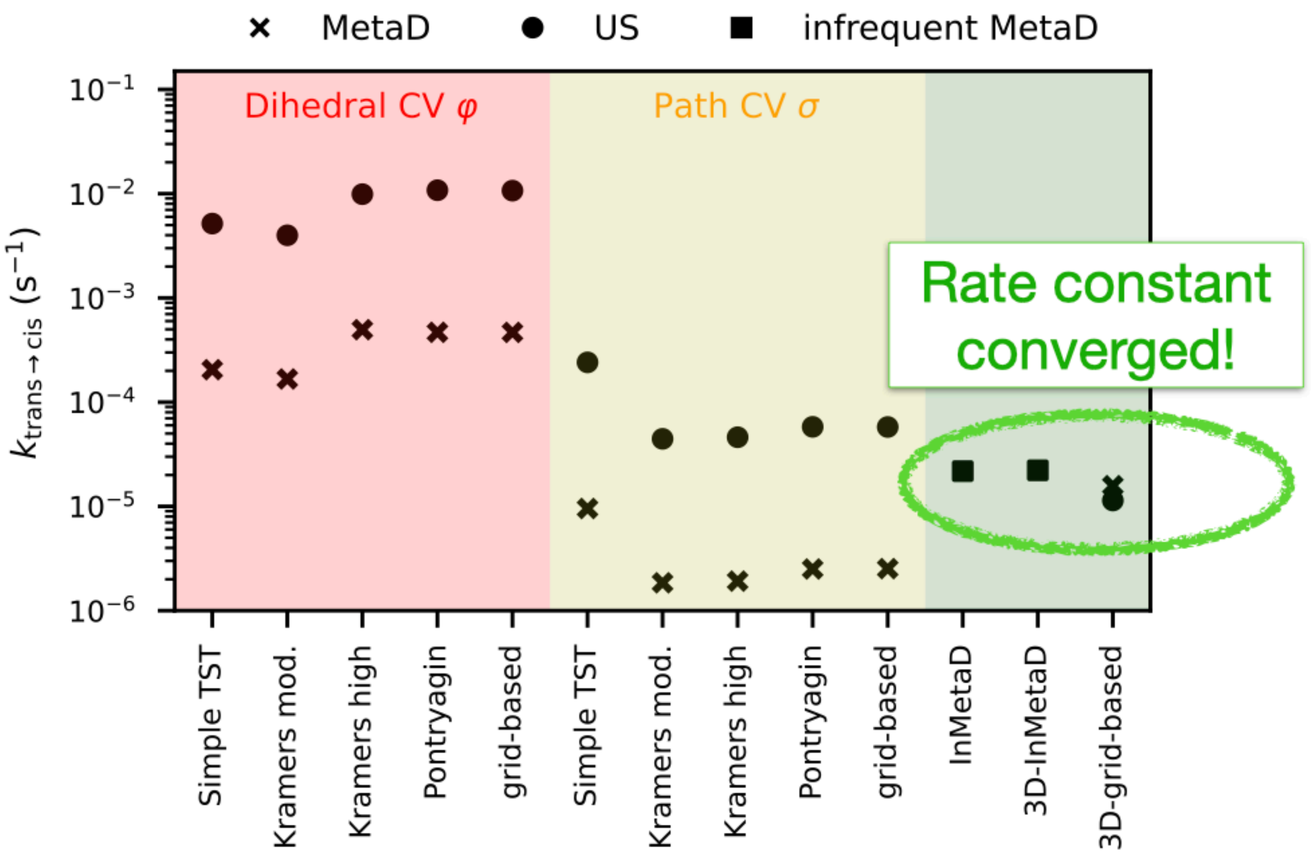


thermal cis-trans isomerization in retinal

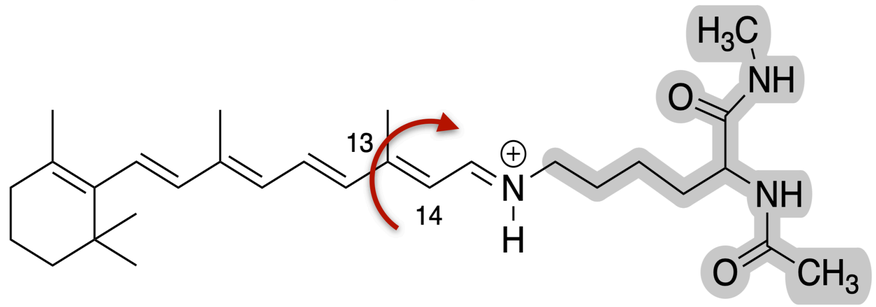


B.G. Keller, P.G. Bolhuis. "Dynamical reweighting for biased rare event simulations." *Annual Review of Physical Chemistry* 75.1 (2024): 137-162.

Simulating chemical reactions

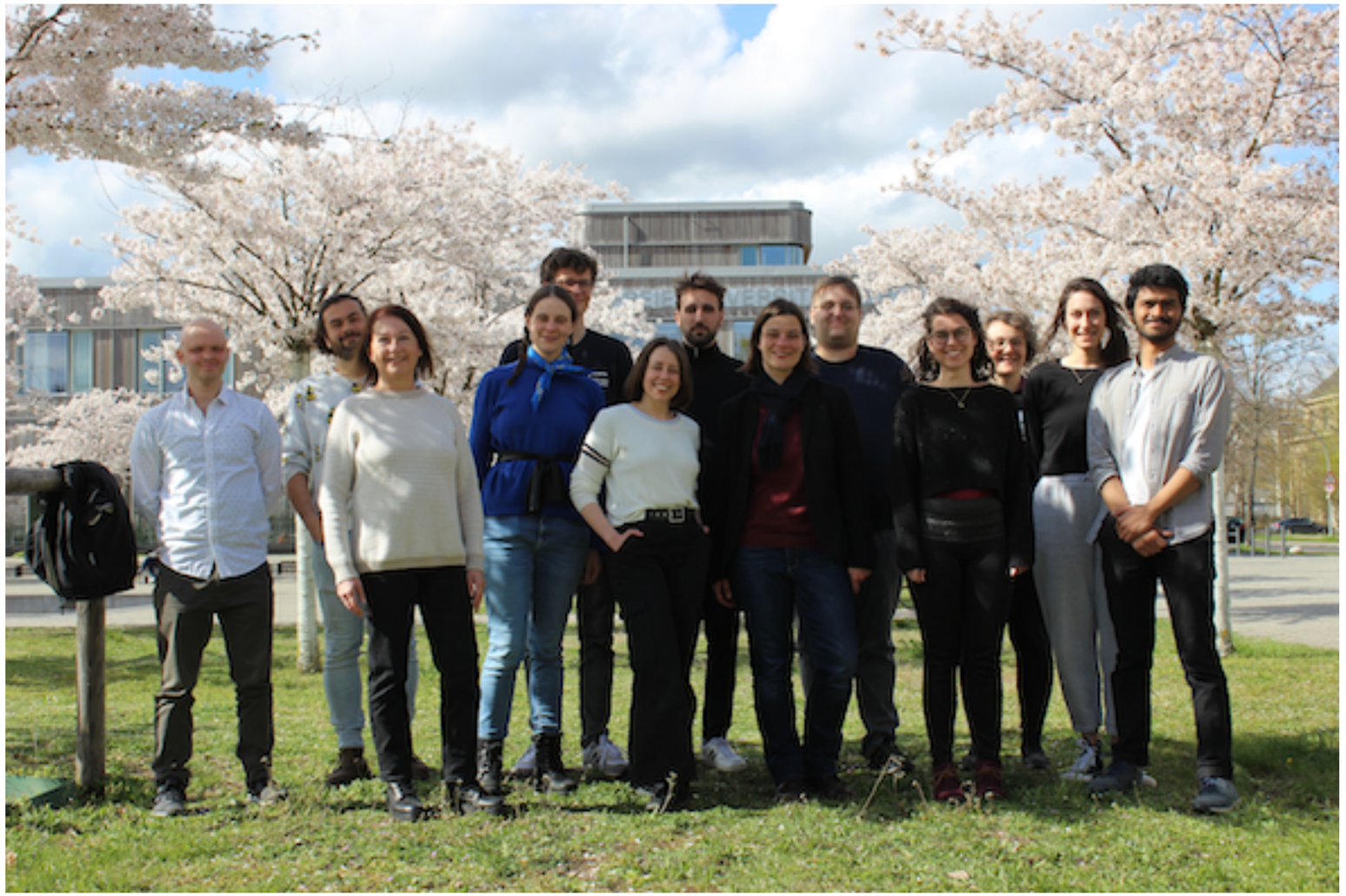


thermal cis-trans isomerization in retinal



S. Ghysbrecht, L. Donati, B.G. Keller "Accuracy of reaction coordinate based rate theories for modelling chemical reactions: insights from the thermal isomerization in retinal"
J. Comput. Chem. (accepted), arXiv https://arxiv.org/abs/2312.12948

Keller group



Group members

- Lauren Finn
- Nikolas Froböse
- Simon Ghysbrecht
- Frederick Heinz
- Sascha Jähnigen
- Leon Werhahn
- Joana-Lysiane Schäfer
- Hana Zupan

Master students and student assistants

- Dominik Dusza
- Aryna Hreben
- Johann Arthur Laux
- Chandramouli Reddy

Thesis or research project

You should have completed on of these courses:

Theoretical Chemistry
Molecular Dynamics

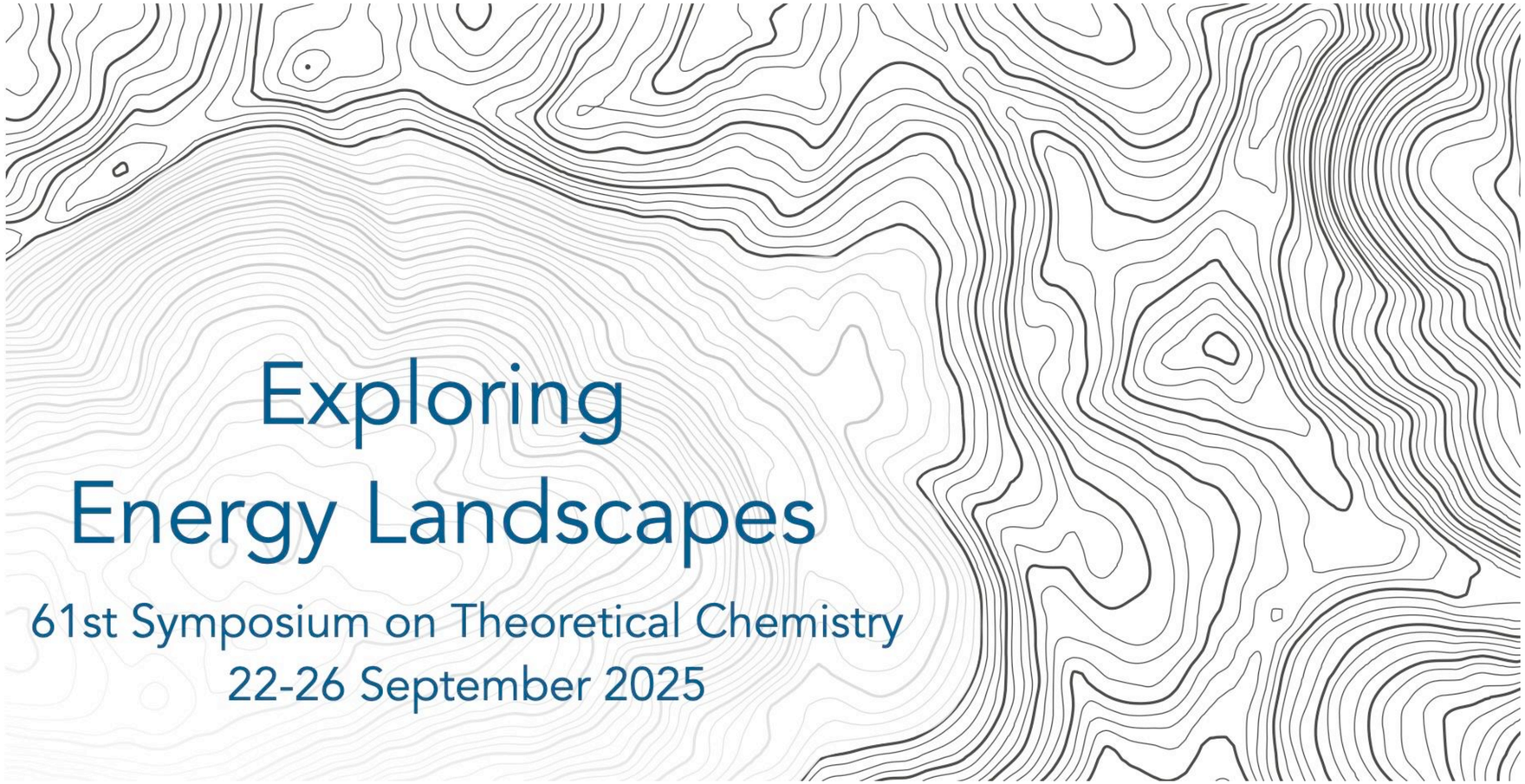
Statistical Mechanics
Quantum Chemistry
DFT

and/or have

Programming experience

Send an email with your background in Theoretical and Physical Chemistry (e.g. transcript of records) to
bettina.keller@fu-berlin.de

61st Symposium for Theoretical Chemistry



Organizers: Bettina Keller, Beate Paulus