Photodynamics of **Acetylacetone** studied by **MeV-UED** *and* the **Berkson's paradox**

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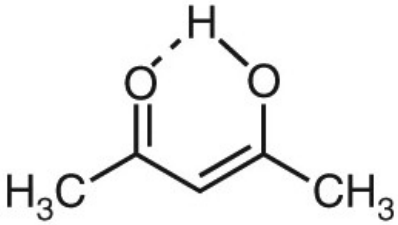
Skilizium-2025

Acetylacetone



> 96 % @ 300 K

UV-Vis: Nakanishi et al. (1977)

Gas-phase ^{1}H NMR: Folkendt et al. (1985)

MW: Caminati et al. (2006)

GED: Lowrey et al. (1971), Iijima et al. (1987), Belova et al. (2014)

UED: Xu, Zewail et al. (2004) [30 kV, $\delta t \approx 2$ ps]

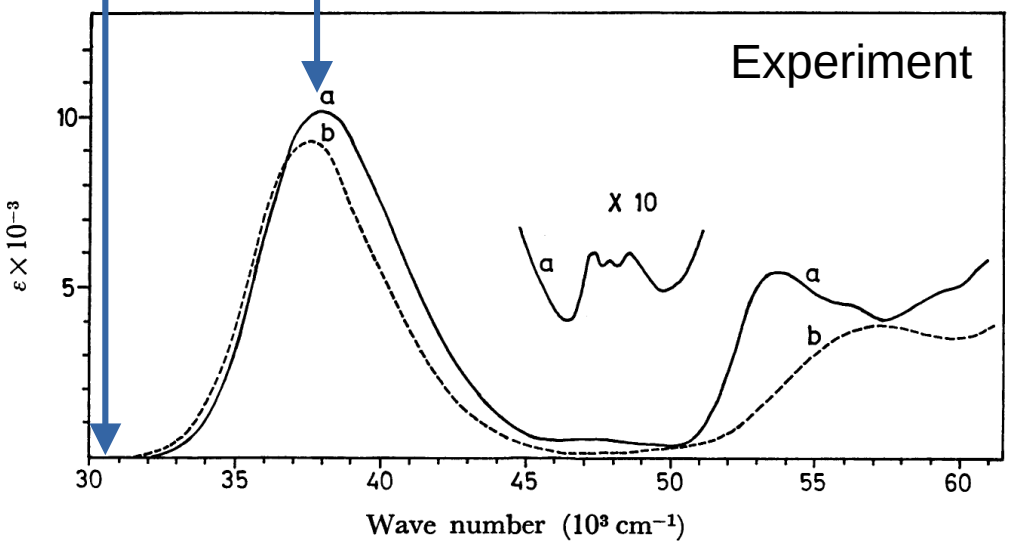
Pump-probe XPS: Bhattacherjee et al. (2017)

Pump-probe PES: Squibb et al. (2018), Kotsina et al. (2020)

Acetylacetone: excited states

S_1 (n, π*) ← S_0

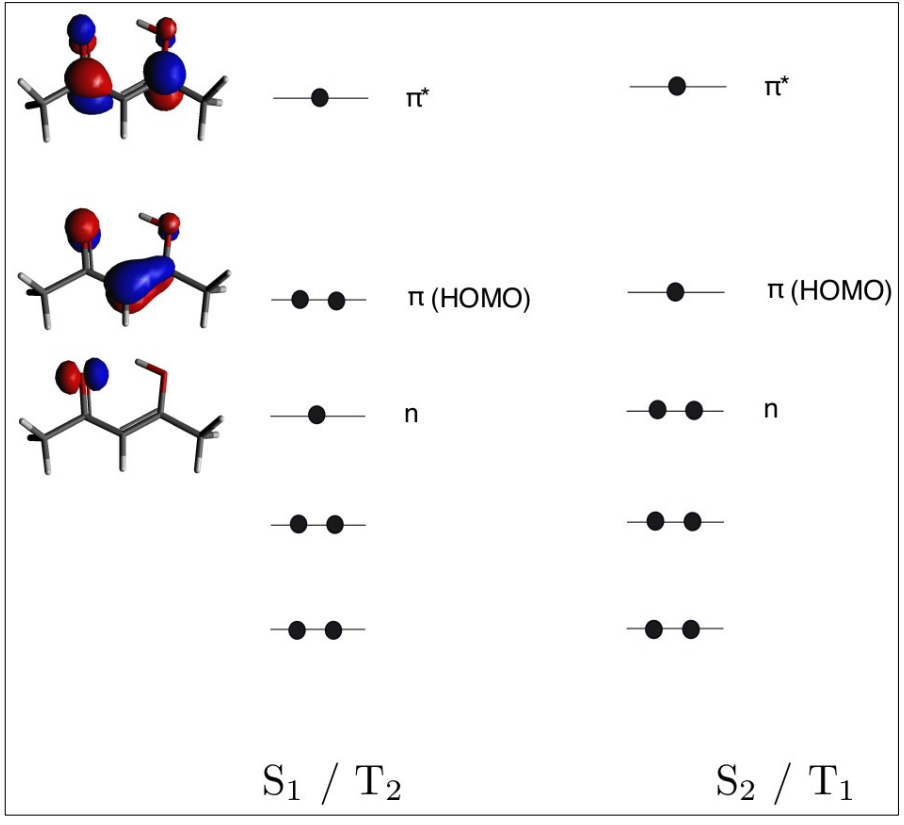
S_2 (π, π*) ← S_0



333 nm 250 nm 200 nm 167 nm

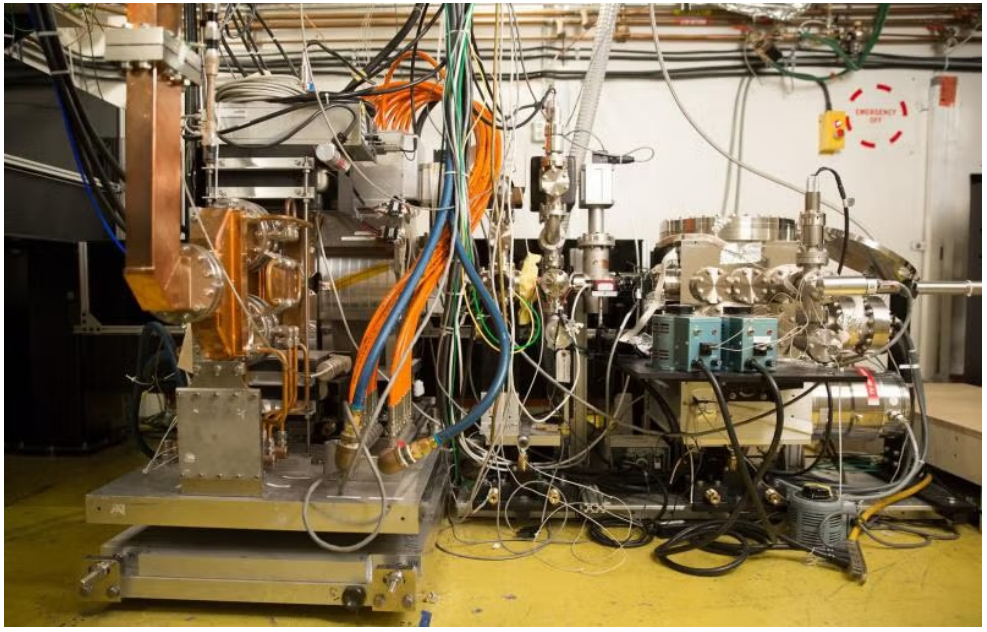
Nakanishi et al., *Bull. Chem. Soc. Jpn.* 1977, 50, 2255.

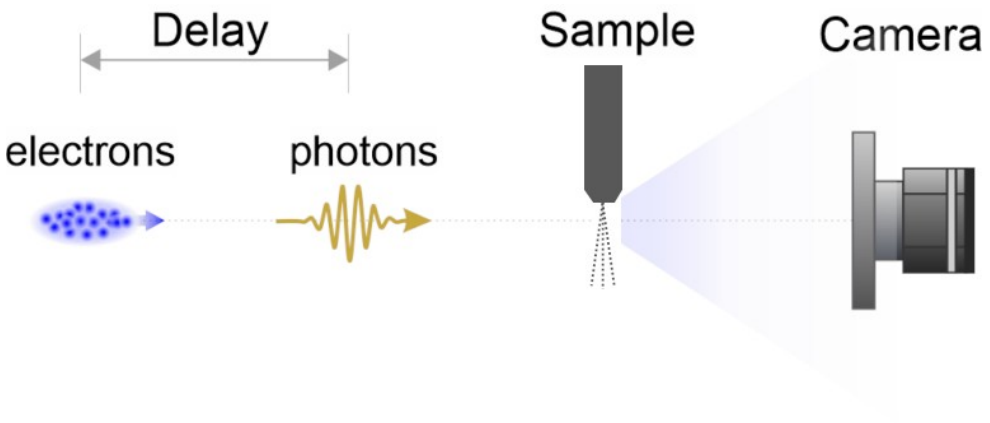
Modell



Ponzi et al., *Molecules* 2022, 27, 1811.

The Instrument: MeV-UED (SLAC – Stanford)

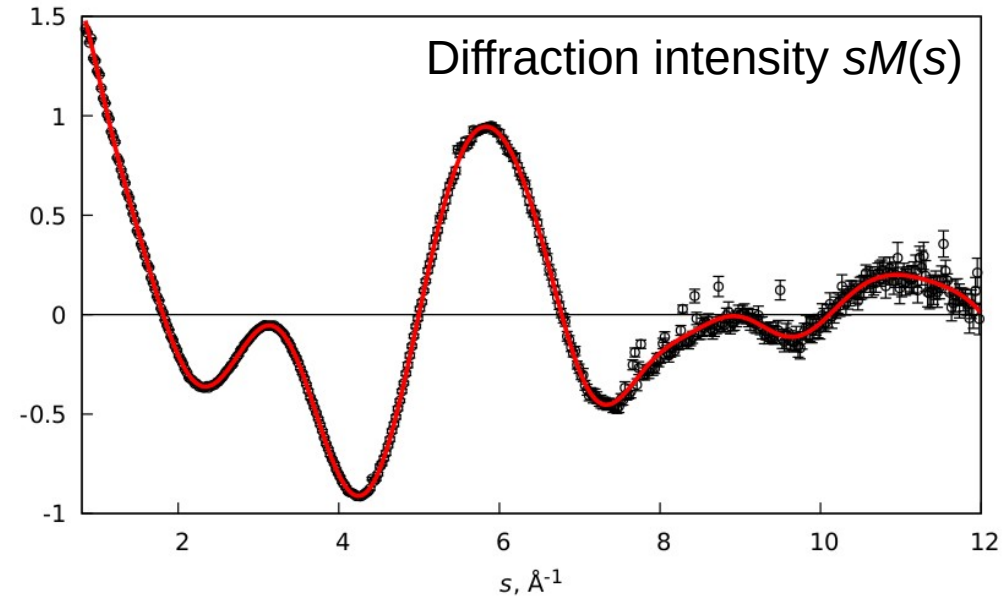


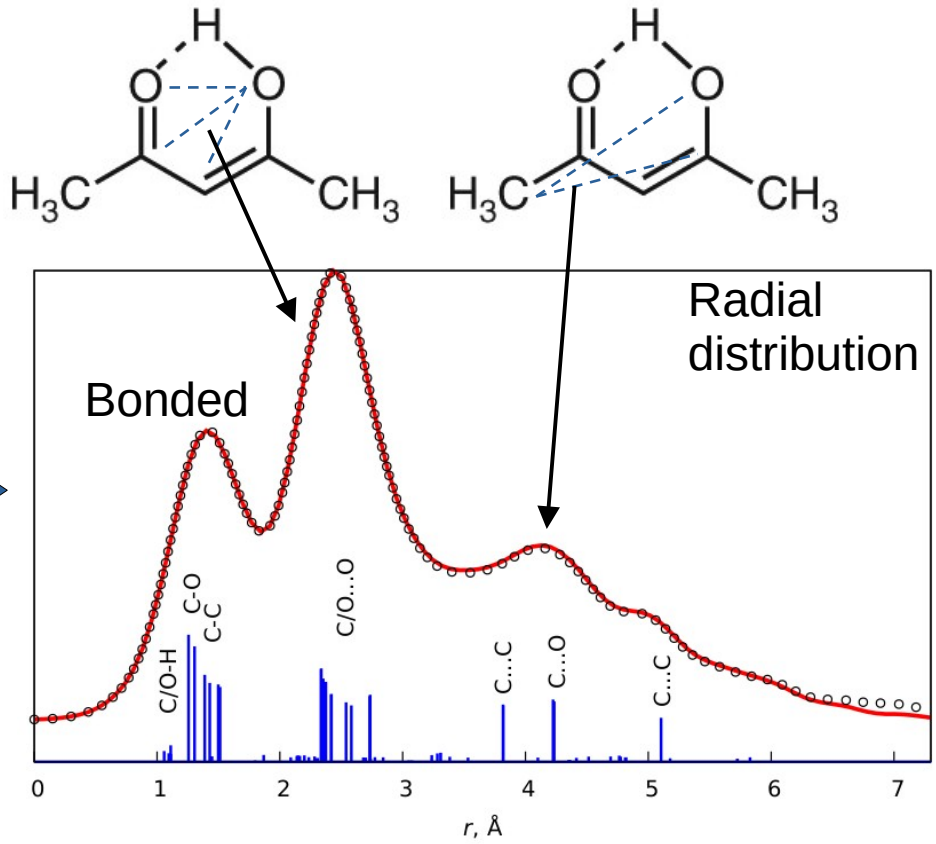


	GED, Bielefeld	MeV-UED, SLAC
e-Energy	60 keV	3.7 MeV = 3700 keV
e-Wavelength	0.05 Å	0.003 Å
e-Speed	0.45 ×*c*	0.9926 ×*c*
e-Mass	1.1 ×m_e	8.24 ×m_e

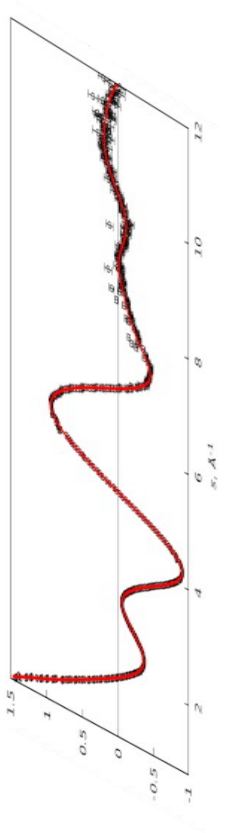
Experimental data @ *dt* < 0

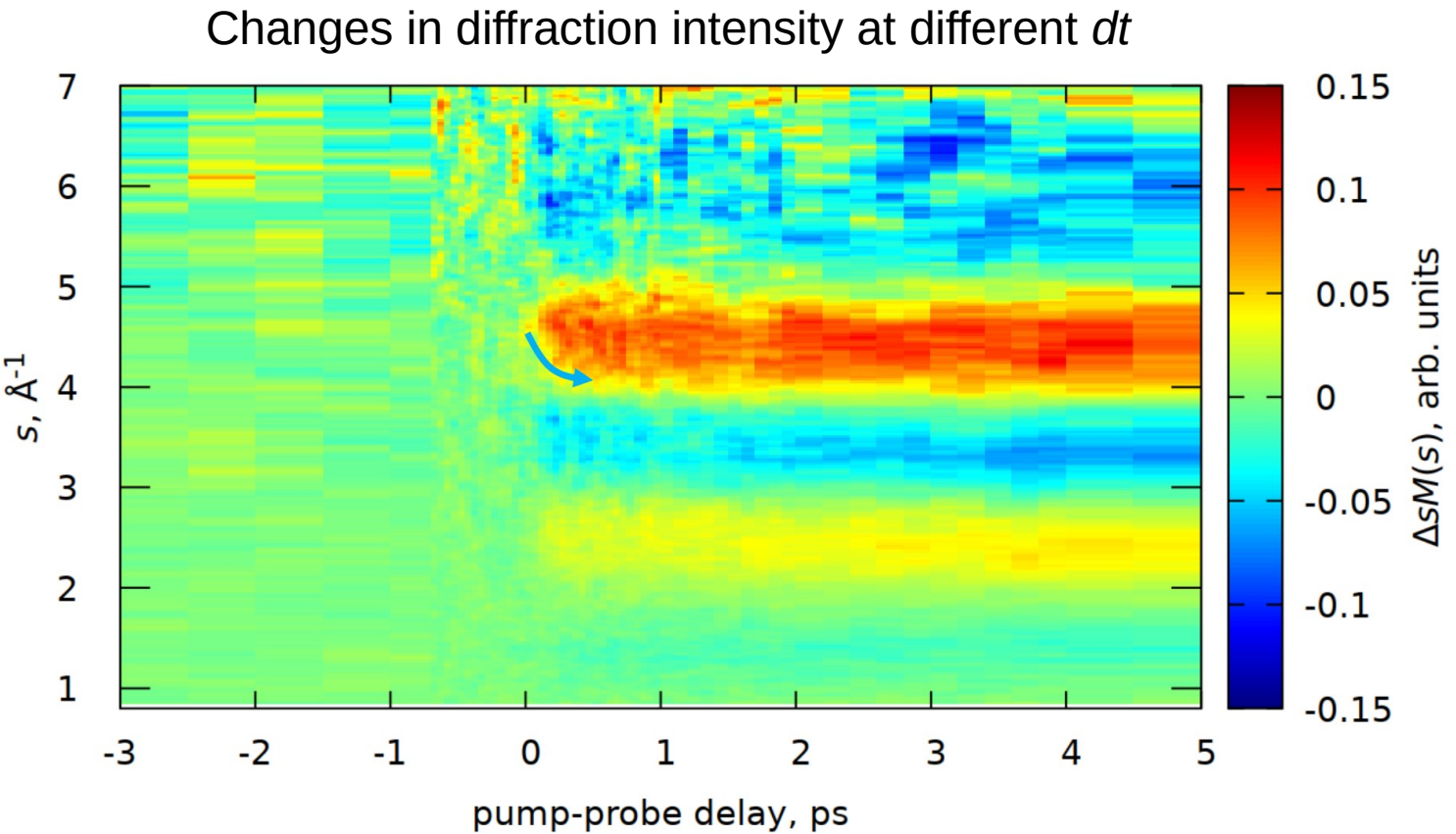
Molecules are in S_0 state!





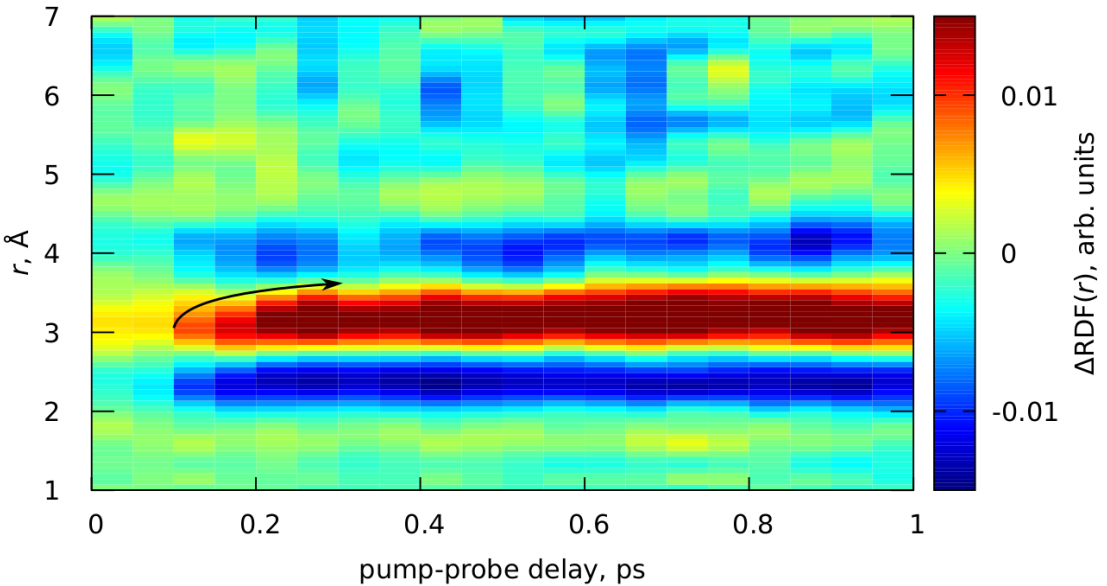
Experimental intensity for *dt* = -3 … 5 ps

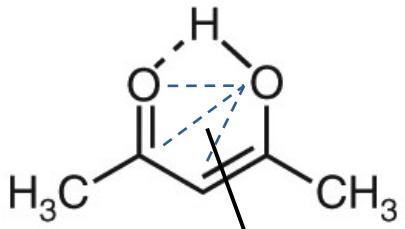




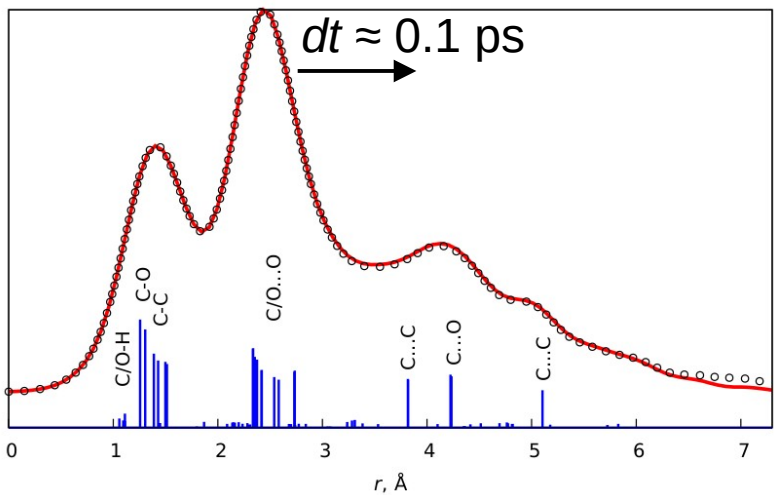
Experimental RDF for *dt* = 0 … 1 ps

Changes in radial distribution function at different *dt*





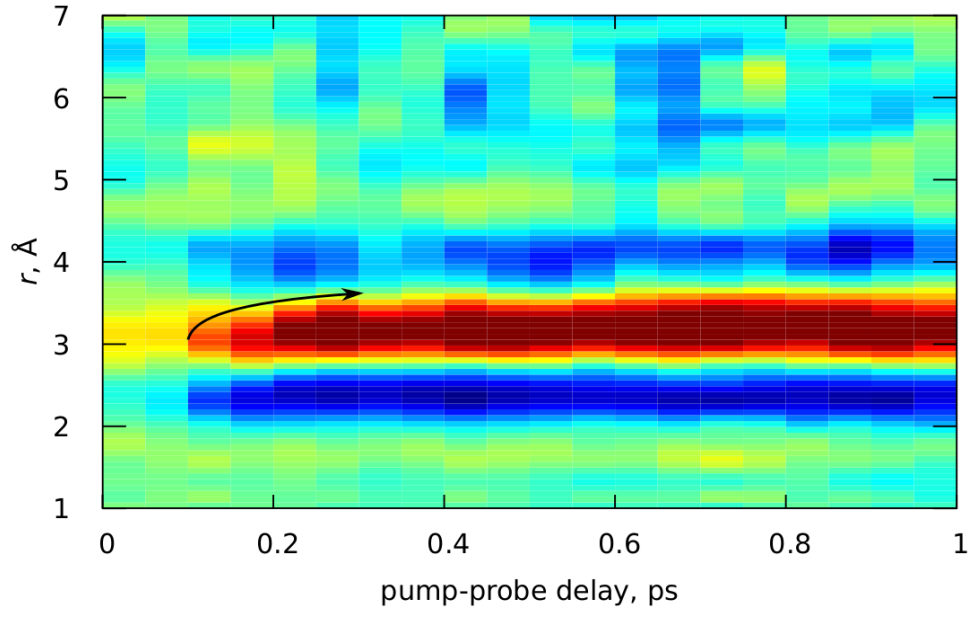
Ring opening after 0.1 ps

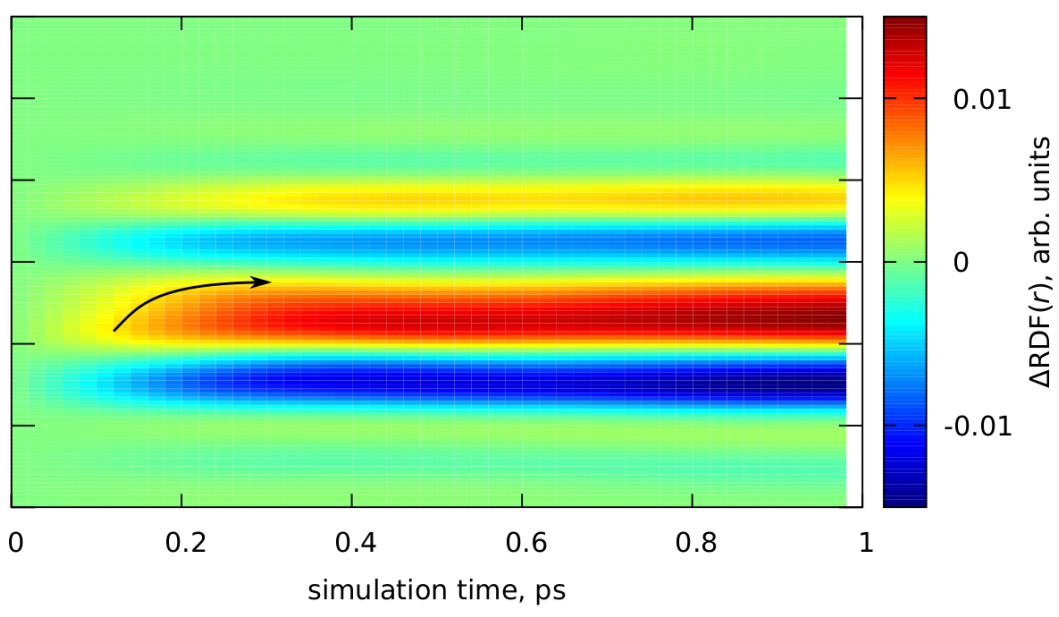


Changes in radial distribution function

Experiment

Model: Nonadiabatic surface hopping simulations

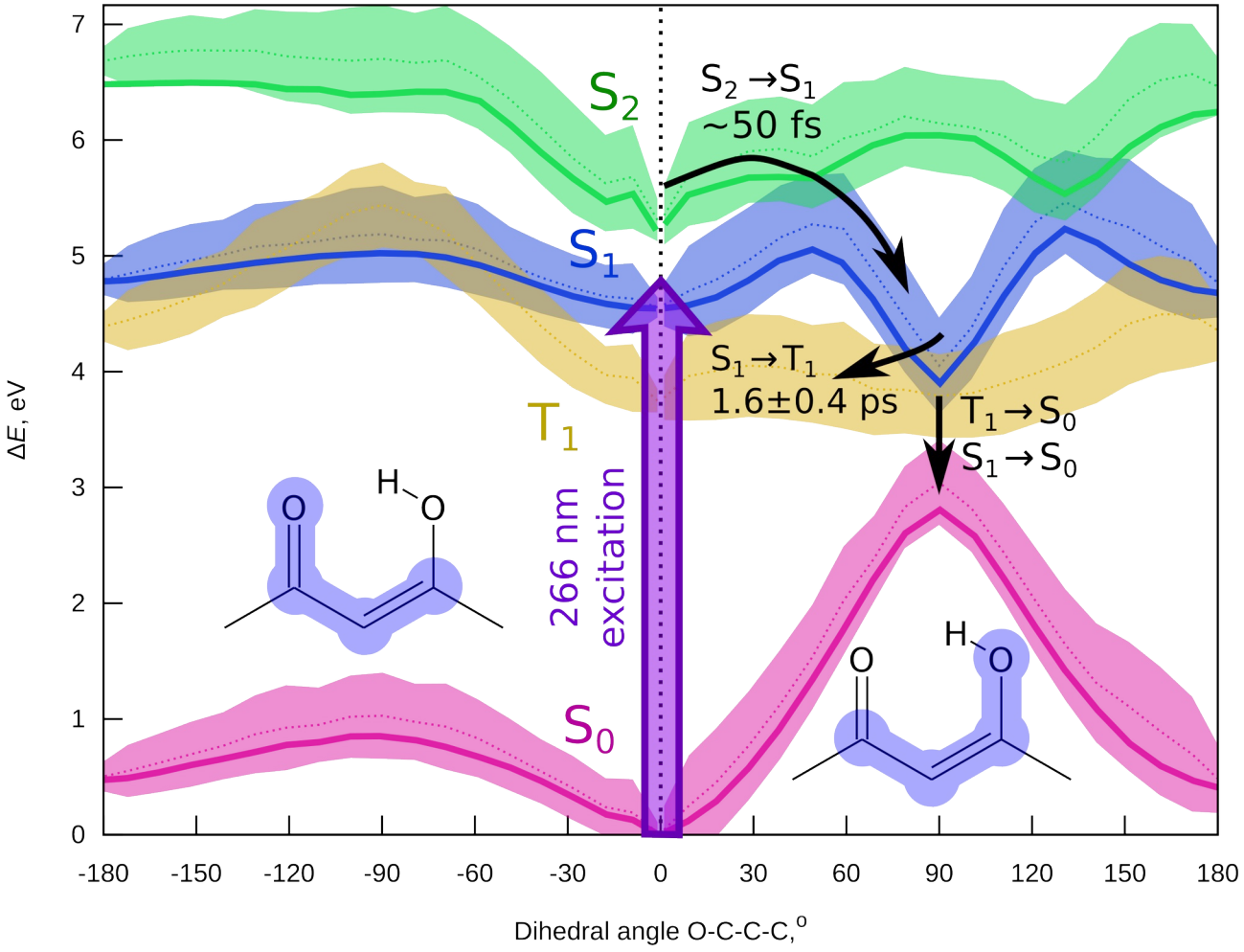




Simulations and results

MeV-UED:

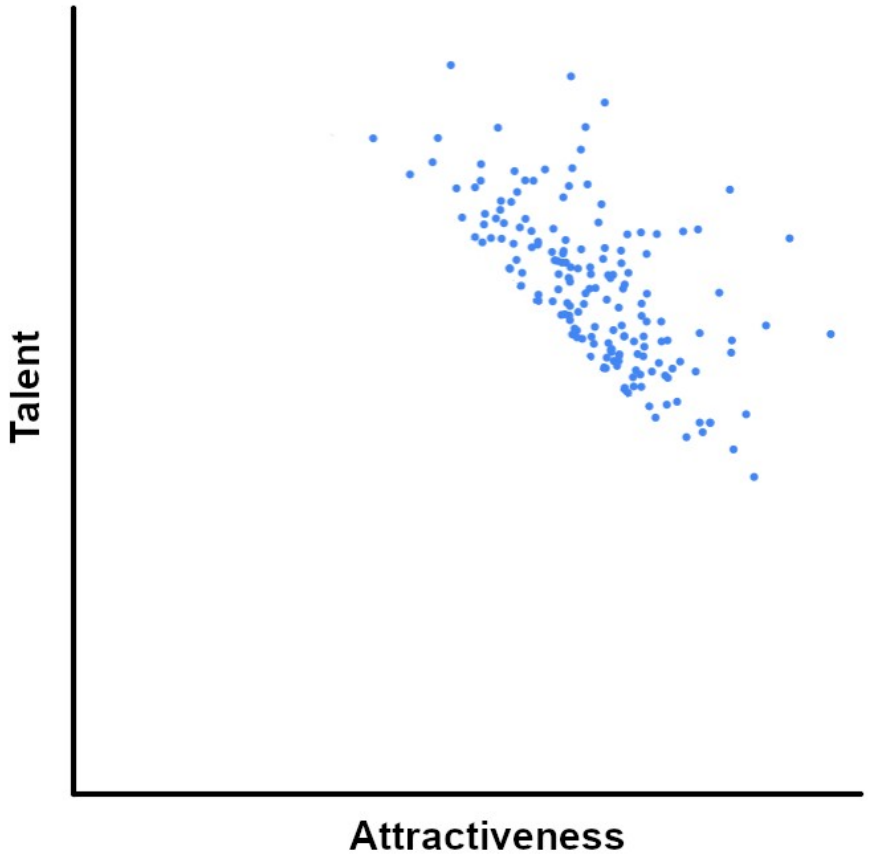
Ring-opening
with characteristic time
≈ 0.7±0.2 ps
is observed in the S_1 state.



The Berkson's paradox

False observation of a **negative correlation** between two desirable traits.

Observed everywhere (!!!), for example:



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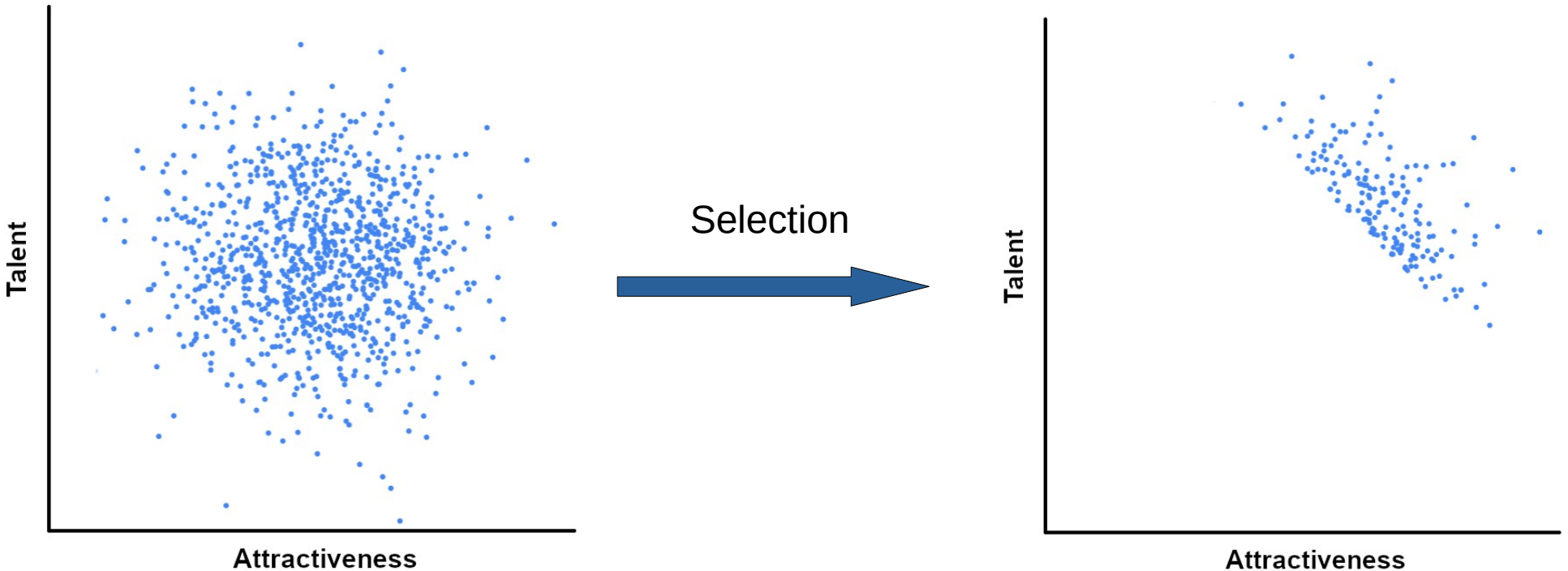
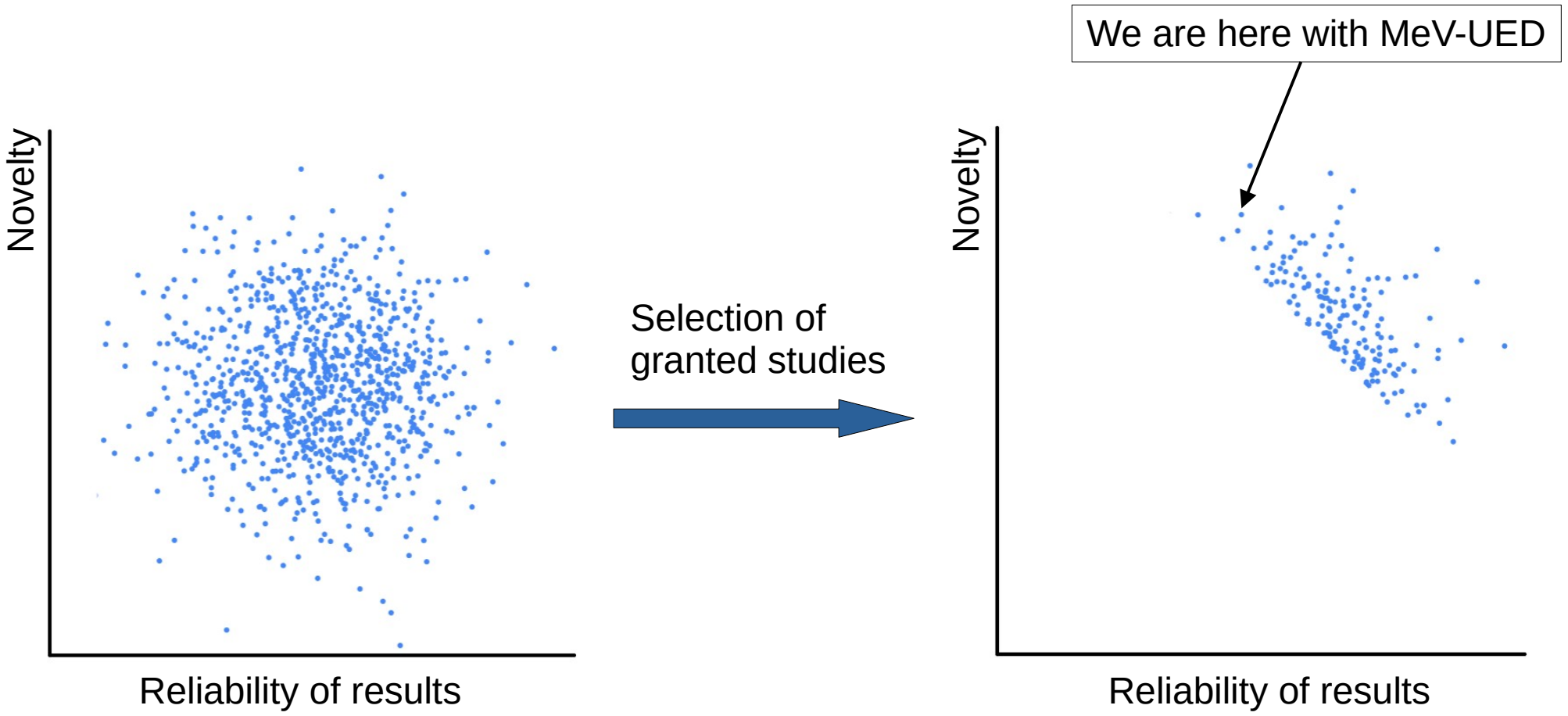


In application to science



Questions?