



Showcasing research in the Wales group at Cambridge University UK.

Analysis and interpretation of first passage time distributions featuring rare events

We develop theory and associated computational tools to investigate the kinetics of competing pathways on multifunnel energy landscapes. Multifunnel landscapes are associated with molecular switches and multifunctional materials, and are expected to exhibit multiple relaxation time scales. We describe a method to produce computationally tractable system sizes, and show how the first passage time distribution can be accessed for landscapes featuring rare events with a wide range of relaxation times. We show how the distribution depends on initial conditions, and how features can be assigned to specific kinetic traps.

As featured in:



See Esmée J. Woods and David J. Wales, *Phys. Chem. Chem. Phys.*, 2024, **26**, 1640.