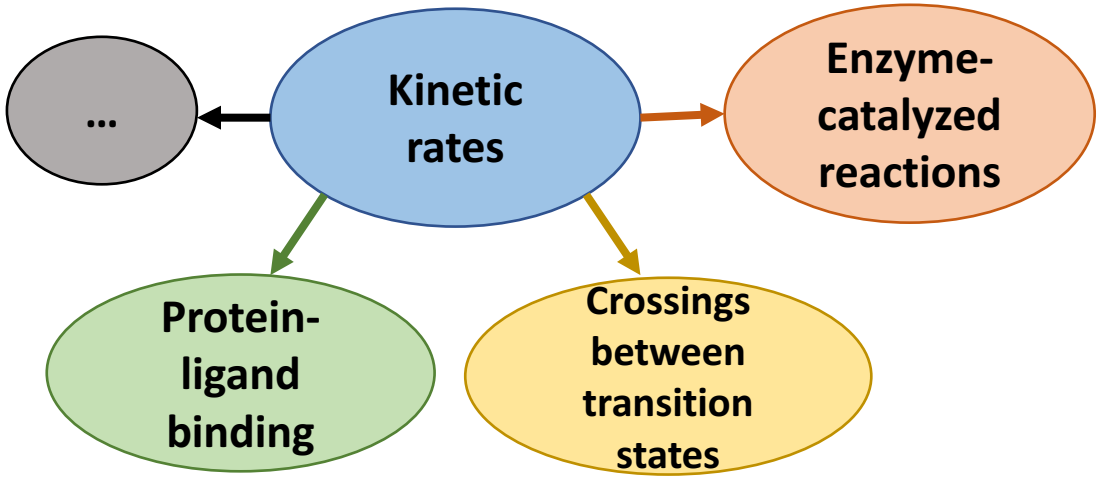
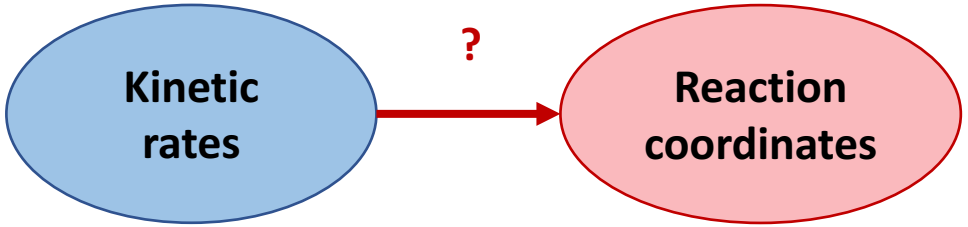
# Collective variable optimization based on kinetic rates




**But what about reaction coordinates?**




**Optimal reaction coordinates yield minimal kinetic rates**







**Proposed method:**
Minimize kinetic rate to obtain optimal RC





W. Zhang, C. Hartmann, and C. Schütte. *Faraday discussions* (2016)

A. Berezhkovskii and A. Szabo. *The Journal of chemical physics* 122.1 (2005).

**L. Mouaffac**, Palacio-Rodriguez & Pietrucci (2023). *arXiv preprint arXiv:2302.12497*

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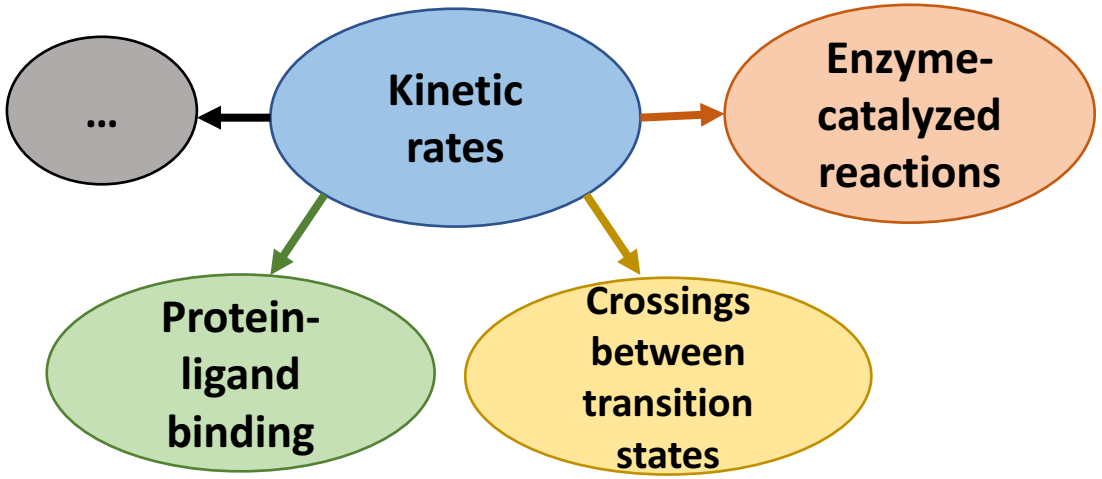
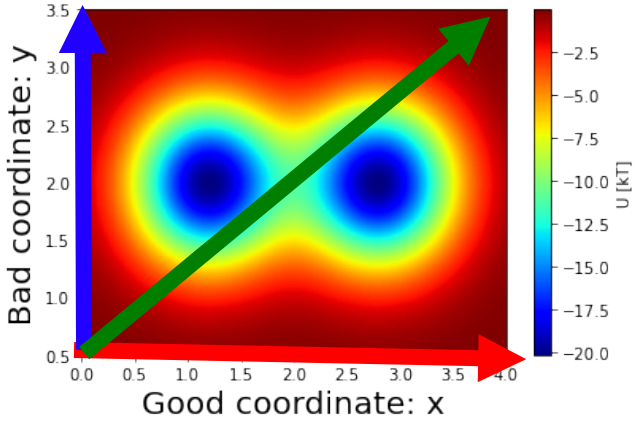
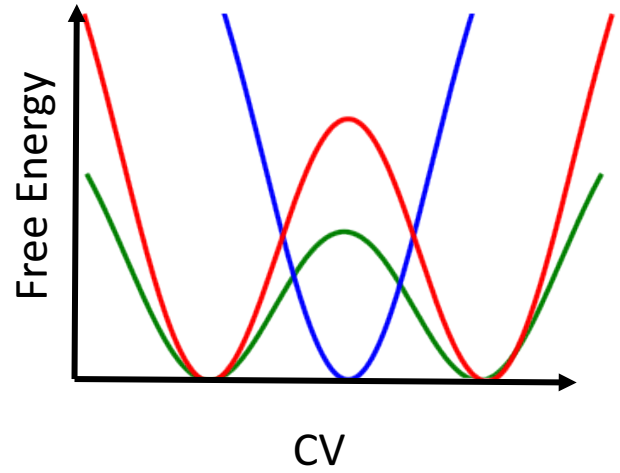



**2D double well**

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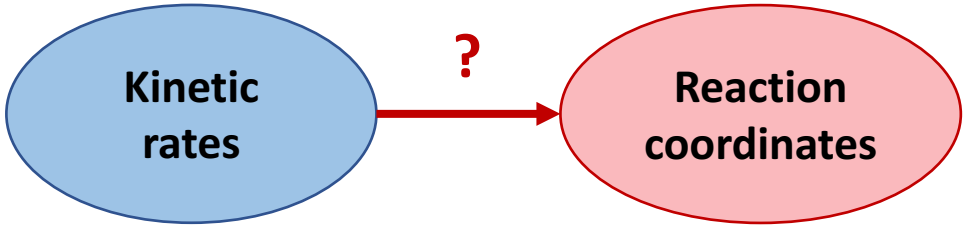
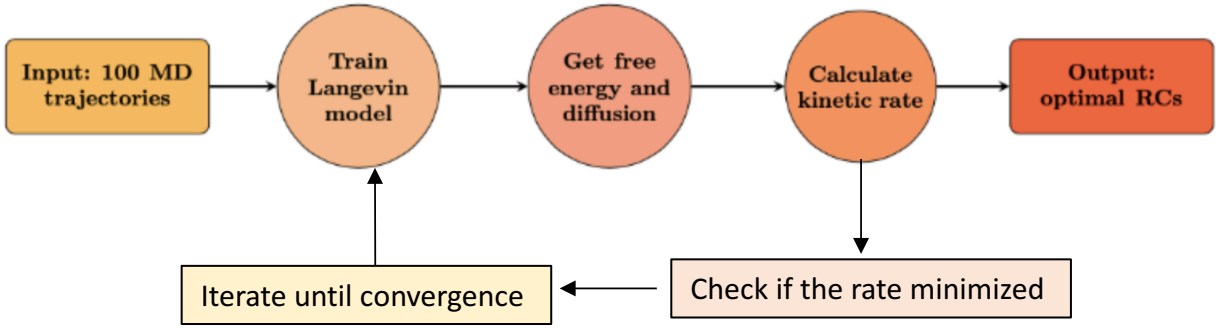



**Optimal reaction coordinates yield minimal kinetic rates**

**Proposed method:**

Minimize kinetic rate to obtain optimal RC





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**L. Mouaffac**, K. Palacio-Rodriguez & F. Pietrucci, *arXiv preprint* (2023)

K. Palacio-Rodriguez & F. Pietrucci, *Journal of Chemical Theory and Computation*, (2022)