UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

Theorie-Kolloquium WS 2023/24
Fr 08.12.2023, 14:00-15:30
MC 351 & online (URL in E-Mail)

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Understanding molecular transitions as pathways in free energy landscapes

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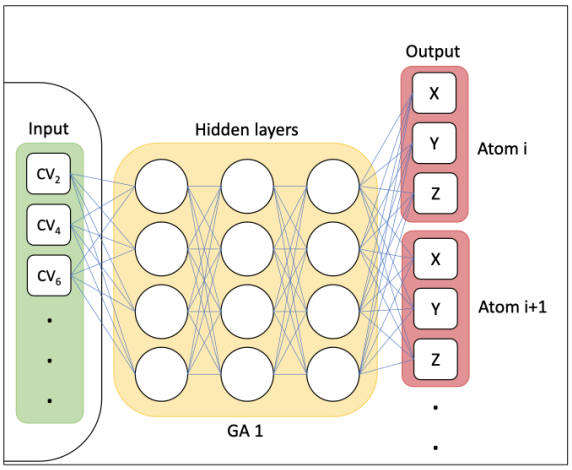

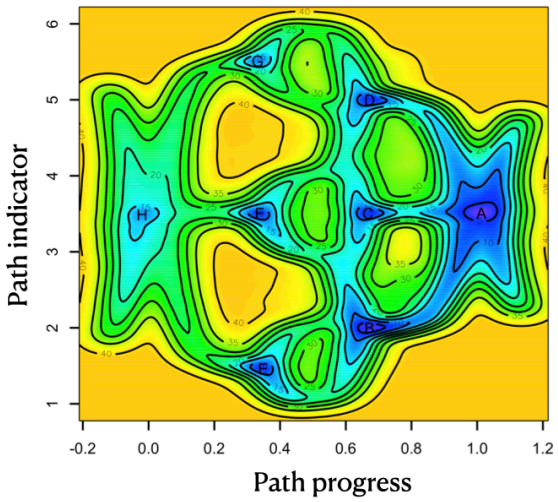

After laying out his momentous contribution to the foundation of quantum mechanics, Paul Dirac allegedly said: "… and the rest is chemistry!". Apparently, Dirac had no idea of the richness and complexity of observable phenomena that emerge as solutions from his Dirac (or Schrödinger's) equation. In this talk, I will showcase several material properties in soft matter and aqueous systems that are, at first sight, remarkably surprising when just regarding the microscopic chemical constituents. Molecular dynamics simulations can be very helpful to unravel the molecular interactions and mechanisms that underly these observable material properties. Molecular transitions, such as chemical reactions, phase transitions, and self-assembly processes can be comprehensibly represented as pathways on low-dimensional free energy landscapes, but this entails finding the essential reaction coordinate(s) or the few collective variables in the many-particle system that describe the molecular process, which is often far from trivial. I will present several in-house developed enhanced sampling methods that we apply for this purpose, including a reinforcement learning approach that does not require prior knowledge of the collective variables [1,2].

[1] Stochastic Optimal Control for Collective Variable Free Sampling of Molecular Transition Paths. NeurIPS (2023)
[2] Advances in enhanced sampling along adaptive paths of collective variables. J. of Chem. Phys. 149, 072320 (2018)