Spice up your computational model with some random numbers: theory and application of the kinetic Monte Carlo method

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Traditionally, first-principles computational chemistry tends to look at chemical reactions from the perspective of energies. In other words, the starting point for investigating a chemical process is, in most cases, the calculation of the reaction and activation energies. However, such data are often not easy to interpret directly. Therefore, it is necessary to use thermodynamic or kinetic models to convert the computed energies into macroscopic observables. However, setting up a model that can be solved analytically is often not trivial, particularly for systems where the reactants are not evenly distributed or have non-negligible interactions with each other. For such cases, one can use a so-called kinetic Monte Carlo (kMC) model, which models a chemical process as a series of stochastic processes.
In this talk, an introduction to the kMC method will be provided. It will then further be shown how such a model has been used to investigate the H_2 storage performance[1] as well as the stability[2] of selected materials. It will be visible that the advantage of the kMC models lies on the one hand in its low computational demand, making it possible to simulate elongated time scales. On the other hand, molecular interactions that are hard to implement in an analytical model can be described relatively easily within the framework of kMC. However, one of the big problems of kMC, namely the strong dependency on the input data and the definition of the model, will also be addressed.

References:

1. T. N.-M. Le, C.-c. Chiu, J.-L. Kuo, *Phys Chem Chem Phys*, **2020**, 22, 4387-4401 DOI: 10.1039/C9CP05796J
2. T. N.-M. Le, C.-c. Chiu, J.-L. Kuo, *Phys Chem Chem Phys*, **in print**, DOI: 10.1039/D1CP02997E

Curriculum Vitae

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Academic Career

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Research interests

Computational chemistry, catalysis, surface science, modeling of thermodynamics and kinetics, modeling of and mass spectrometry