# MolSpin – Introducing a versatile software package for spin chemistry

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Spin-dependent chemical reactions reveal fascinating mechanisms which are of high interest in the current scientific community. For instance, the application of an external magnetic field would affect the yield in simple radical reactions of formic acid formation [1]. Furthermore, spin-dependent reactions are believed to be the fundamental cause for endowing migratory birds with the ability to sense the Earth's magnetic field [2]. It is thus important to understand and describe the dynamics and interactions of spin systems of varied complexity. Not only the interactions between spins but also the influence of the environment exhibits an important aspect which leads to observable effects in experiments. The underlying theoretical framework to describe these effects relies on the Liouville-Von-Neumann equation. However, the solution of this equation is in most cases not only challenging for realistic systems but also requires the utilization of supercomputers.

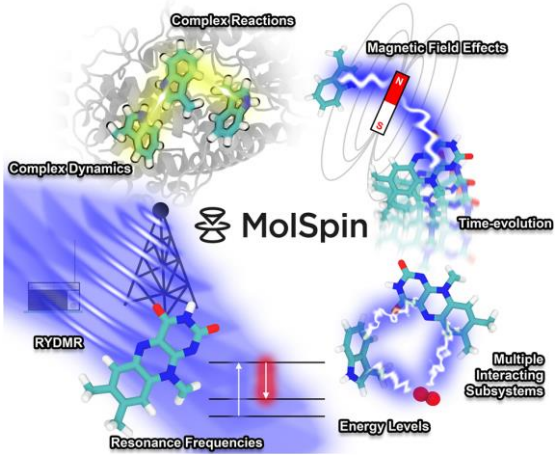


**Figure 1** Examples of problems that can be described by MolSpin [3].

We have developed the software package MolSpin to efficiently solve and investigate spin dynamics for spin chemistry problems [3]. With MolSpin it is possible to describe spin-dependent reaction mechanisms, the influence of molecular motion and other perturbations using the Bloch-Redfield-Wangsness formalism, and several other features. The software package is built to allow for an easy implementation of additional tasks and is thus suitable for challenging problems related to spin dynamics.

[1] T. C. Player, *J. Chem. Phys.*, **153**, 084303 (2020).

[2] J. Xu *et al.*, *Nature*, **594**, 535-540 (2021).

[3] C. Nielsen *et al.*, *J. Chem. Phys.*, **151**, 194105 (2019).