university of groningen

"The research within the Groningen Theoretical Chemistry group focuses on both development and application of hybrid classical/quantum dynamical methods for studies of lightinduced processes and quantum effects in biomolecules and novel materials.

Method development: Very recently, we developed an extremely efficient approach for using machine learning algorithms and methods borrowed from the realm of artificial intelligence to dramatically reduce the cost of excited-state non-adiabatic dynamics. This is a new era and not yet explored in theoretical chemistry, where machine learning and artificial intelligence boost molecular simulations of complex light-induced processes.

Application: In addition to overcoming fundamental challenges in the field, we are pursuing exciting applications such as photo-switchable molecular motors relevant for molecular electronics, photo-switchable DNA used in nanotechnology, singlet fission in molecular solids to increase the efficiency of solar cells, and excited-state processes of far-red fluorescent proteins used in optogenetics.

Other areas of our activity are the development and application of non-orthogonal methods, such as valence bond theory. This method is used to describe bonding in molecules and to describe energy and charge transfer processes. Furthermore, we also develop methods for the calculation of response properties, in particular magnetic response, and apply it to study aromatic molecules. Elucidation of reaction mechanisms of photocatalytic reactions is an application area in which we use our methods that we are developing."