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IWR COLLOQUIUM WINTER SEMESTER 2023/24

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An Interdisciplinary Journey of Computational Mathematics in Theoretical Chemistry

Numerical simulations are widely used as a third pillar besides experimental and theoretical investigations in many sciences such as physics and chemistry as well as engineering science. It requires the development of robust and efficient numerical methods for the resolution of the underlying physical laws that arise often in form of partial differential equations (PDEs). In this talk, I will describe two interdisciplinary stories. While illustrating the key-ideas of the theory and methods, I will also highlight the occasions where not only the mathematical tools have been successfully developed and transferred to the application but also where the interdisciplinary interactions raised new mathematical questions and triggered new answers and theories in mathematics. From the application viewpoint, this talk will touch upon implicit solvation models and Born-Oppenheimer molecular dynamics but the methods rely on various and divers mathematical concepts from Grassmann manifolds to descriptors from machine learning and perturbation theory.

Also streamed via Zoom

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Mathematikon • Conference Room / 5th Floor
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