

Loic Joubert-Doriol and Benjamin Lasorne

(Université Gustave Eiffel, Paris /
Institut Charles Gerhardt Montpellier)

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Introduction to Modelling Molecular Observables and Spectral Responses

TUM Garching, Boltzmannstr. 3,
85748 Garching Forschungszentrum, room 03.10.011

Abstract: This talk will provide a partial overview of how to model molecular observables and spectral responses.

We shall start with the essential quantum mechanical concepts and formalisms that are used in theoretical chemistry and molecular physics.

This will be followed by an illustration of the tools that are involved in numerical simulations in this context.