

Module title		Abbreviation
Theoretical Models in Chemistry		o8-TC-092-m01
Module coordinator		Module offered by
lecturer of lecture "Quantenchemie"		Institute of Physical and Theoretical Chemistry
ECTS	Method of grading	Only after succ. compl. of module(s)
3	numerical grade	--
Duration	Module level	Other prerequisites
1 semester	undergraduate	Admission prerequisite to assessment: successful completion of exercises in the respective classes as specified at the beginning of the course (usually 70% of exercises to be successfully completed) as well as regular attendance of exercises (usually a maximum of 2 incidents of unexcused absence).
Contents		
This module provides students with deeper insights into advanced topics in quantum chemistry. It focuses on spin, the Pauli principle, Slater determinants, the Hartree-Fock method, correlation energy, configuration interaction and excited states, the Born-Oppenheimer approximation and bonding models of H ₂ ⁺ .		
Intended learning outcomes		
Students are able to describe excited states of molecules with the help of key concepts and models.		
Courses (type, number of weekly contact hours, language – if other than German)		
V + Ü (no information on SWS (weekly contact hours) and course language available)		
Method of assessment (type, scope, language – if other than German, examination offered – if not every semester, information on whether module is creditable for bonus)		
a) 1 to 3 written examinations (1 written examination: approx. 90 minutes; 2 written examinations: approx. 60 or 90 minutes each; 3 written examinations: approx. 60 minutes each) or b) oral examination of one candidate each (approx. 20 minutes) or c) oral examination in groups (groups of 2, approx. 30 minutes)		
Allocation of places		
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Additional information		
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Workload		
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Teaching cycle		
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Referred to in LPO I (examination regulations for teaching-degree programmes)		
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Module appears in		
Bachelor' degree (1 major) Chemistry (2010) Bachelor' degree (1 major) Chemistry (2009) Bachelor' degree (1 major) Mathematics (2012) Bachelor' degree (1 major) Mathematics (2013) Bachelor' degree (1 major) Computational Mathematics (2009) Bachelor' degree (1 major) Computational Mathematics (2012) Bachelor' degree (1 major) Computational Mathematics (2013) Bachelor' degree (1 major) FOKUS Chemistry (2011)		