

Module title		Abbreviation
Theoretical Models in Chemistry		o8-TC-o72-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	--
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: 90 minutes; 2 written examinations: 60 or 90 minutes each; 3 written examinations: 60 minutes each) or b) 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 (2007)		
Bachelor' degree (1 major) Mathematics (2007)		