

<b>Module title</b>		<b>Abbreviation</b>
Theoretical Models in Chemistry		o8-TC-141-m01
<b>Module coordinator</b>		<b>Module offered by</b>
lecturer of lecture "Quantenchemie"		Institute of Physical and Theoretical Chemistry
<b>ECTS</b>	<b>Method of grading</b>	<b>Only after succ. compl. of module(s)</b>
3	numerical grade	--
<b>Duration</b>	<b>Module level</b>	<b>Other prerequisites</b>
1 semester	undergraduate	--
<b>Contents</b>		
<p>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<sub>2</sub><sup>+</sup>.</p>		
<b>Intended learning outcomes</b>		
Students are able to describe excited states of molecules with the help of key concepts and models.		
<b>Courses</b> (type, number of weekly contact hours, language – if other than German)		
V + Ü (no information on SWS (weekly contact hours) and course language available)		
<b>Method of assessment</b> (type, scope, language – if other than German, examination offered – if not every semester, information on whether module is creditable for bonus)		
written examination (approx. 90 to 180 minutes) or oral examination of one candidate each (approx. 20 to 30 minutes) or oral examination in groups (groups of 2, approx. 30 minutes) Language of assessment: German, English		
<b>Allocation of places</b>		
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<b>Additional information</b>		
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<b>Workload</b>		
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<b>Teaching cycle</b>		
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<b>Referred to in LPO I</b> (examination regulations for teaching-degree programmes)		
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<b>Module appears in</b>		
Bachelor' degree (1 major) Mathematics (2014)		
Bachelor' degree (1 major) Computational Mathematics (2014)		