Presentation of the WP 4 (QC II)
“Advanced Quantum Chemistry Methods” (SS 2020)

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01/23/2020
Presentation of the WP 4 (QC II)

“Advanced Quantum Chemistry Methods”

see: https://www.chemie.uni-bonn.de/pctc/mulliken-center/teaching/qc2/quantum-chemistry-ii + eCampus course

- lecture “QC II”: **Tue. 1:15-2:45 pm**, seminar room 0.005 (MCTC), Beringstr.4; start: **04/07/2020**
- prerequisites for participation
  - passed modul MCh 1.4 (“QC 1”)
- seminar
  - own seminar talk (Thu. 8-12 am, topics and exact dates will be fixed later)
  - recommended attendance of the TC colloquium (Thu. 5:15-6:15 pm)
- achievements necessary to qualify for the module’s examination
  - passing the practical course (protocol)
  - seminar talk about a recent scientific publication
- examination
  - oral exam (end of July / mid August)
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practical course: (organization: Sebastian Spicher spicher@thch.uni-bonn.de)

1. programming in Fortran: implementation of a Hartree-Fock and UHF or MP2 program
(tutors: Sebastian Ehlert, Philipp Pracht, Sebastian Spicher)
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2. application of quantum chemical programs to solve chemical questions (thermochemistry, kinetics, spectroscopy)
(tutors: Sebastian Spicher, Sarah Schmitz, Julius Stückrath)

- attendance time: **Thu. 8-12 am**, independent working possible during the whole semester in the computer rooms of the MCTC (Beringstr. 4, room 2.008 and 3.007)
- registration until **03/02/2020**: hansen@thch.uni-bonn.de
- preliminary meeting: **Tue. 04/07/2020, 12:45 am** (before the 1st lecture), seminar room 0.005 (MCTC), Beringstr.4