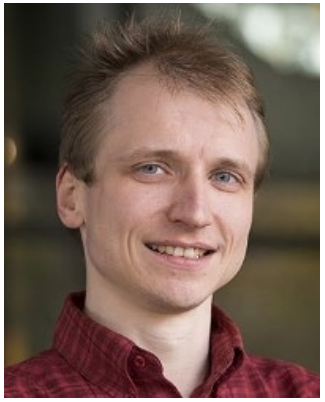
Theoretical Chemistry (1/2)



Universiteit Leiden

VU HG-13A33
Thu, 30-01-25, 10.00 – 12.00

- From the foundations to practical DFT calculations:
  - The Kohn-Sham approach
  - Exchange-correlation functionals
  - “Putting it on a computer” (basis sets & and some other implementation details)

Theoretical Chemistry (2/2)

- Description versus Understanding in Theoretical Chemistry
- Activation Strain Model (ASM) of chemical reactivity
- Canonical Energy Decomposition Analysis (EDA) in the context of Kohn-Sham MO Theory - Factors determining Bond activation catalysis
- Steric nature of the Bite-Angle effect
- Electronic Regime versus Electronic Configuration
- Pauli-lowering catalysis

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