Material thermal, electrical and optical properties; A multiscale approach from atom scale to engineering scale.

Research institution

Université de Lorraine – LEMTA

Research team

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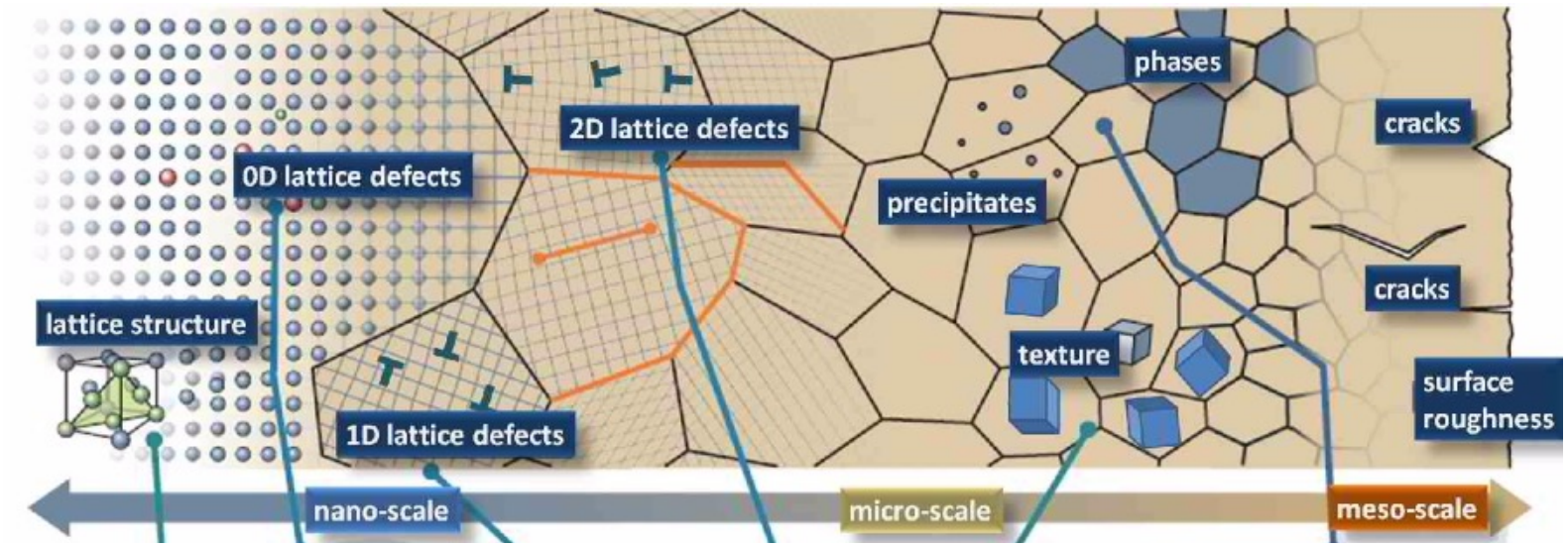
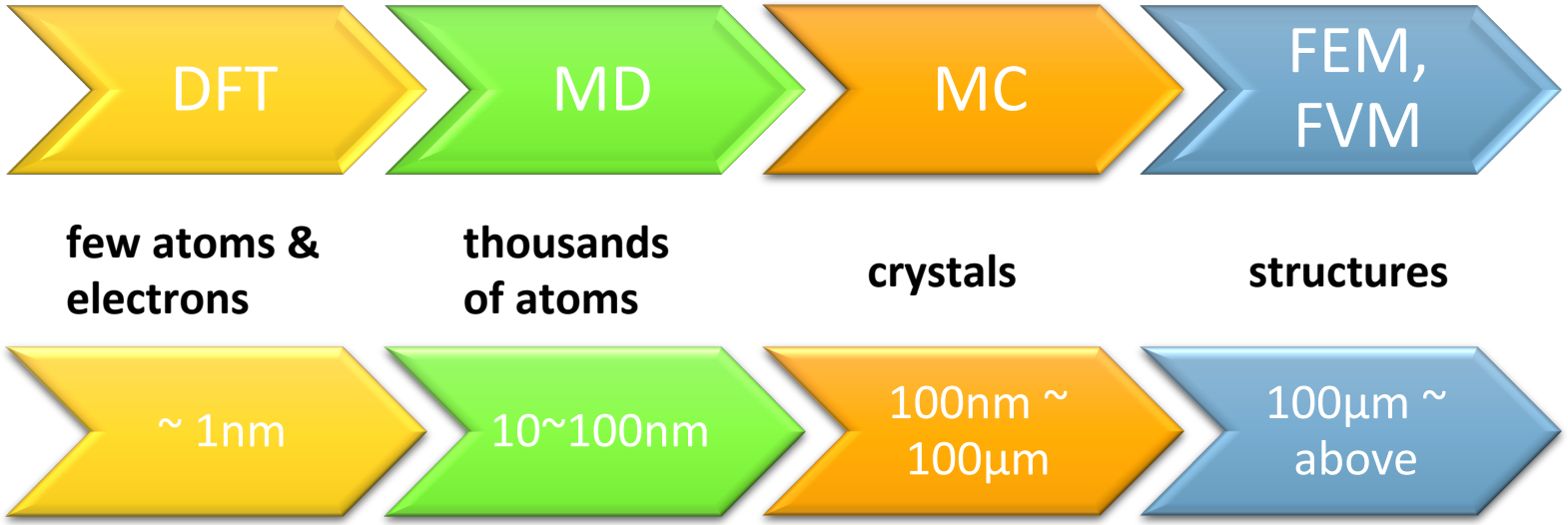
Transport property modeling and characterization: a multiscale expertise





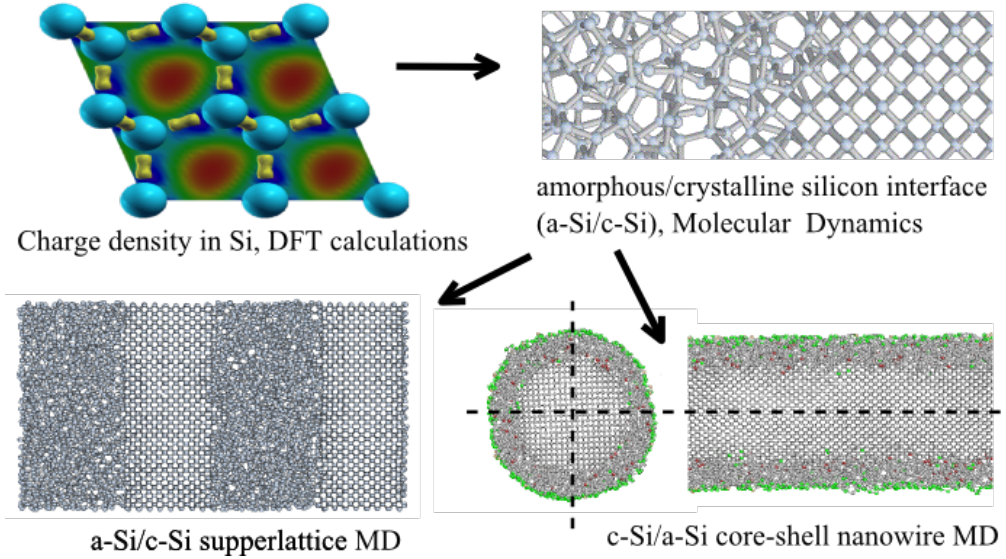
LEMTA investigates material properties at multi-scales ranging from the primitive cell to the device structure.

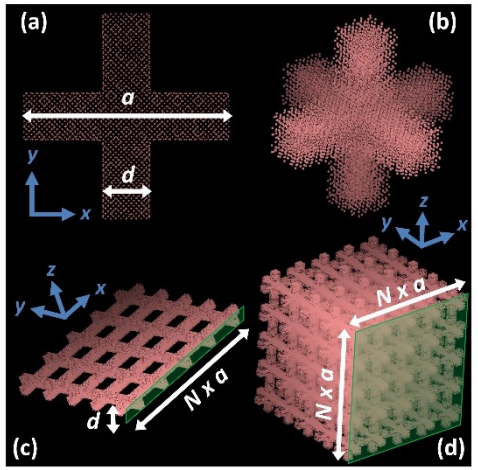
Areas of expertise are conjugated **simulations** (*DFT, MD, MC, FEM*) and **experiments** (*SThM, FDTR, Raman & FTIR spectroscopies*)

http://www.dierk-raabe.com/

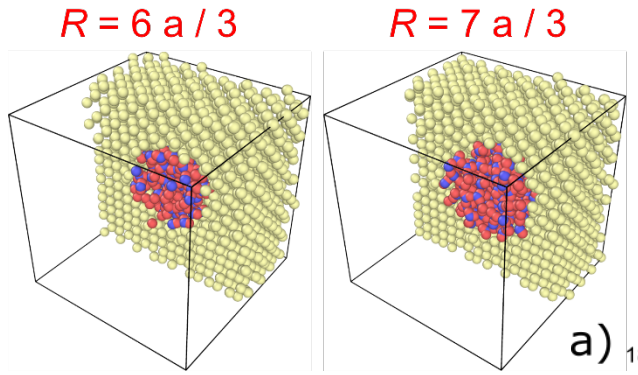
Small scale models and tools for material design

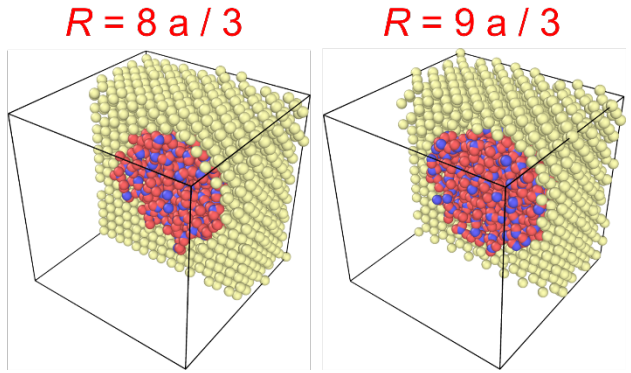
- Small scale modelling is fundamental to **study and predict** physical properties of materials.
- The latter one can be obtained with quantum mechanics using ***ab-initio* methods.**



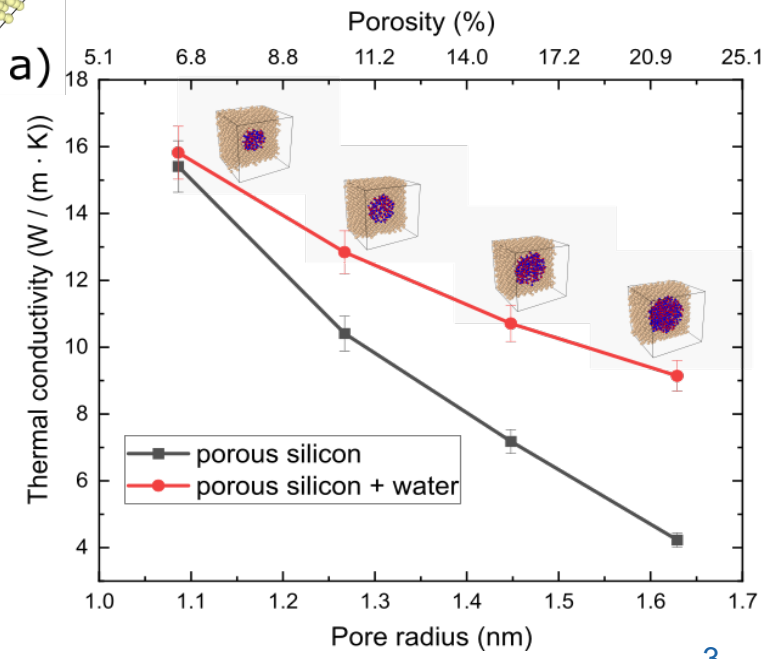


Application of DFT and MD to silicon based materials

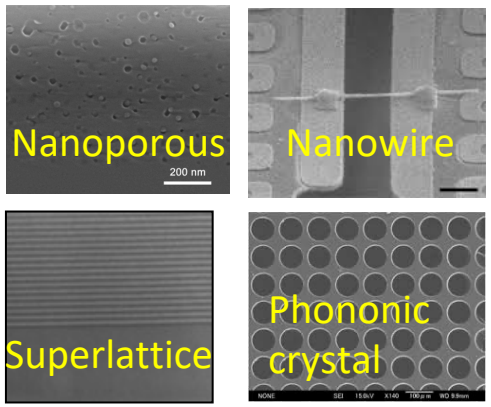




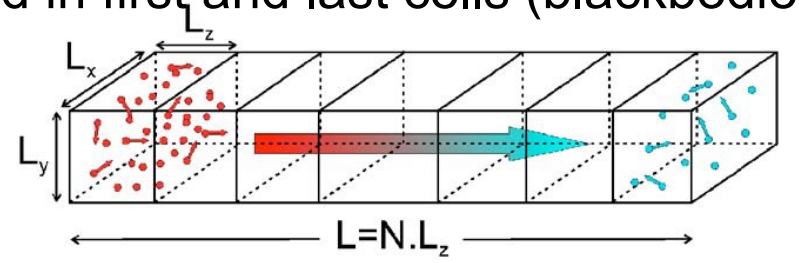
Porous silicon with and without water molecules filling



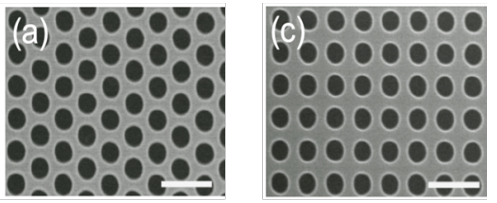
Monte Carlo solution of the BTE



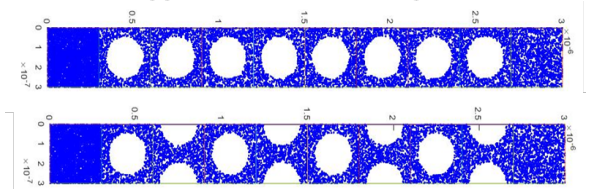
Structures are discretized taking into account periodicities, temperature are prescribed in first and last cells (blackbodies)

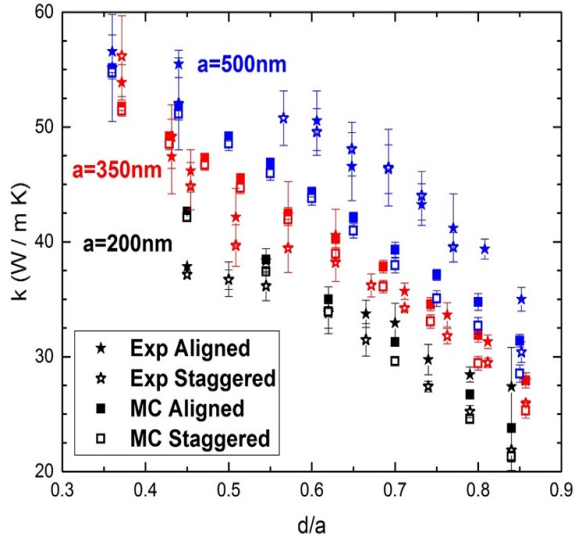


Phononic Si membranes

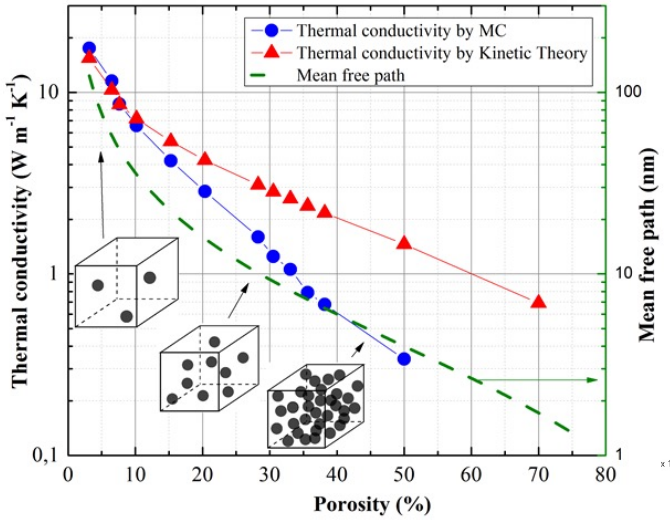


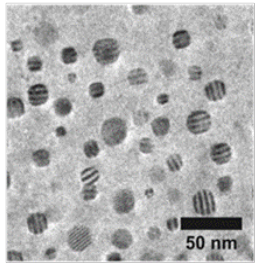
'Staggered' 'Aligned'

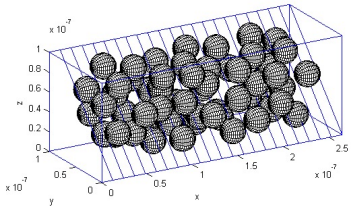




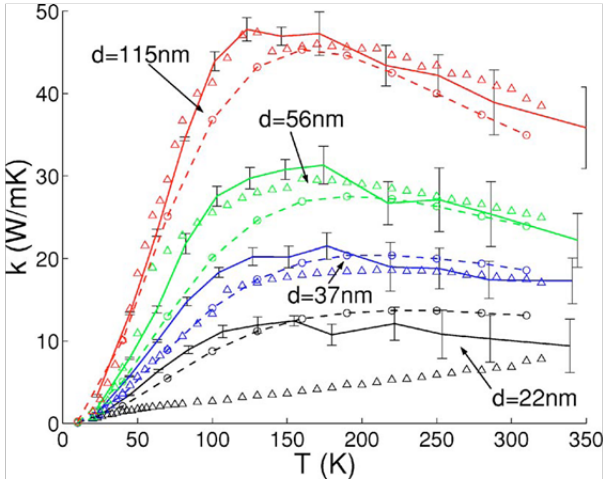
Porous membranes/membranes with inclusions

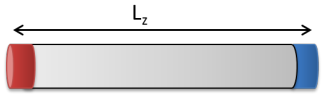






Si nanowire thermal conductivity vs temperature



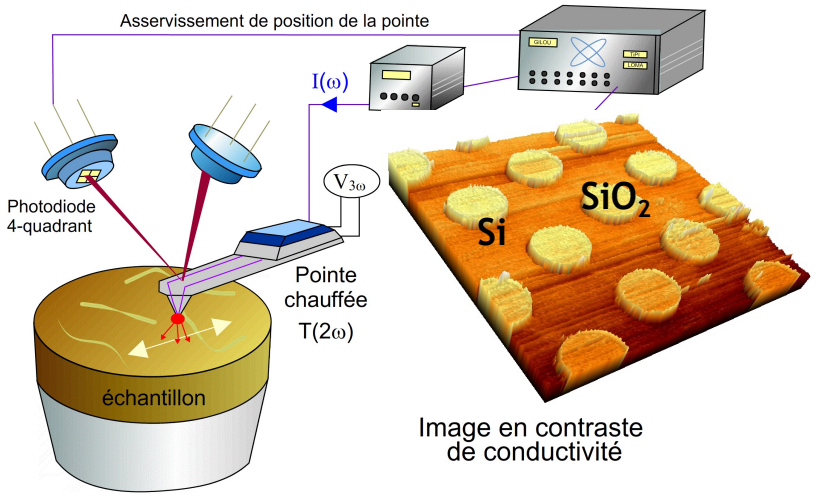


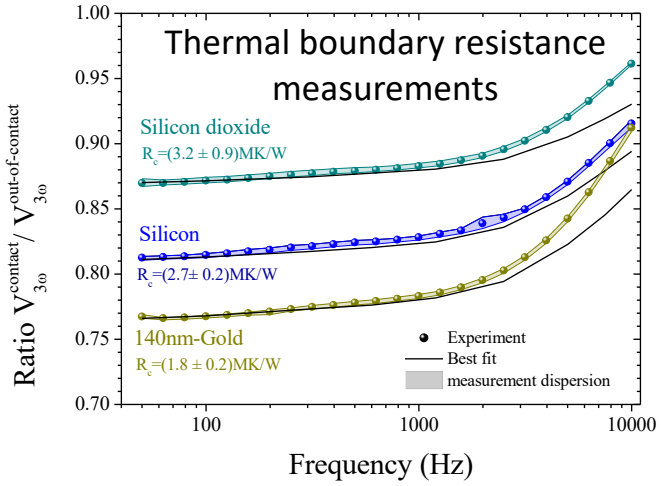
Smooth nanowire

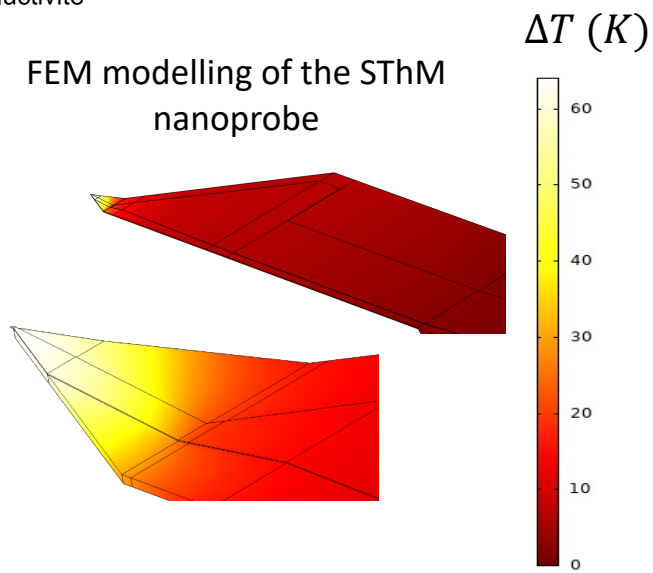
Experimental approaches

❑ 3ω-Scanning Thermal Microscopy

- Spatial resolution: {50-100}nm
- Temperature sensitivity : mK



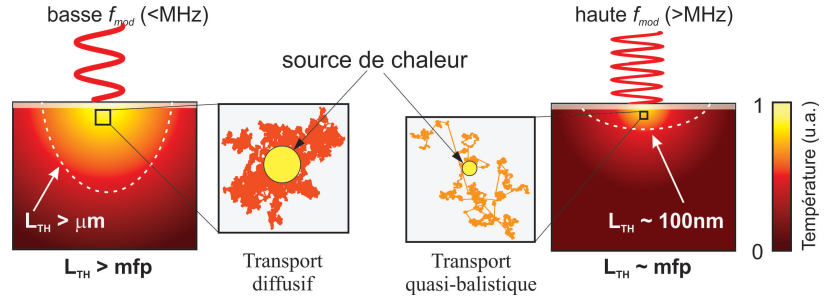




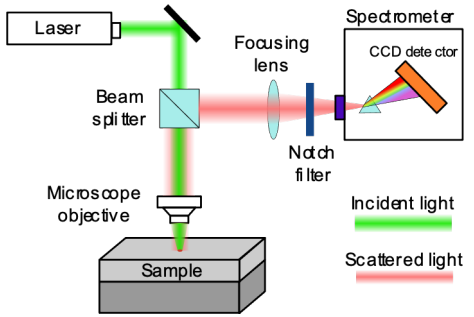
OPTICAL APPROACHES

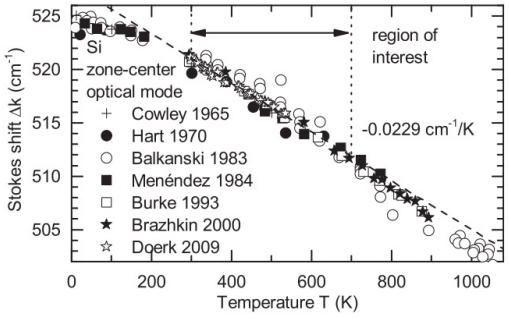
❑ Frequency Domain Thermoreflectance

- Wide range of frequencies [10kHz-100MHz]
- Ballistic-diffusive heat transfer



❑ Raman Spectroscopy





❑ Photoacoustic method (in development)

Teams – Alumni & collaborations

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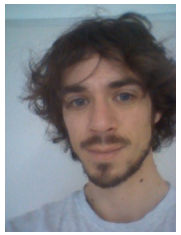

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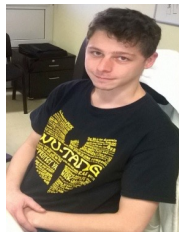

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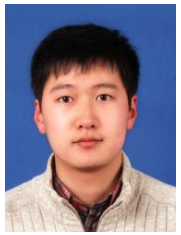

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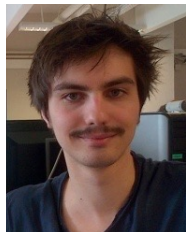

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