

Topic 5: high throughput and correlated magnetic resonance for increased information density

Vlad Badilita, Neil MacKinnon



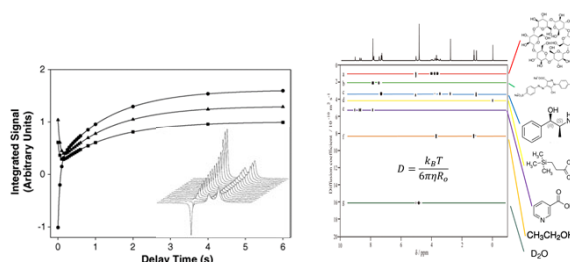
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Information provided by magnetic resonance

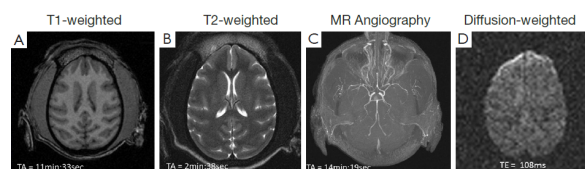
■ Spectroscopy

- Molecular structure
- Chemical exchange (intra-, intermolecular)
- Molecular transport (diffusion, flow)
- Physical parameters (pH, T, hydrophilicity, binding)



■ Imaging

- Spatial distribution of nuclear spin
- Contrast encoding based on physical parameters (density, T_1 , T_2 , diffusion, flow)

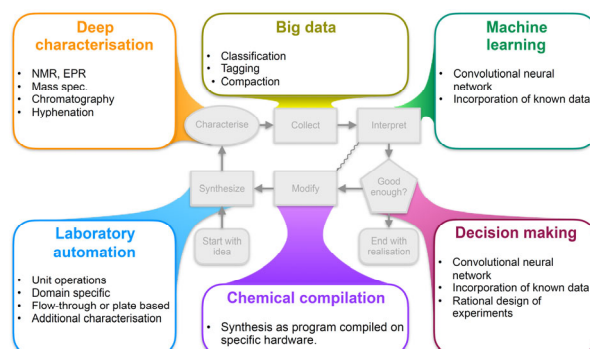


■ Imaging + spectroscopy: localized information

Xiaodong Zhang, et al., *Quantitative Imaging in Medicine and Surgery* 4 (2014) 112

HiT-NMR: high throughput screening

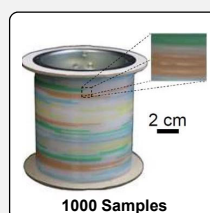
- Standard NMR measurements are done serially
- Measurement acceleration will be achieved by
 - Plug-flow based sampling approach
 - Parallelization of measurement sites
- Increased data volume will be used for machine-assisted sample preparation



The HiT-NMR lab @ IMT

Automation scheduling

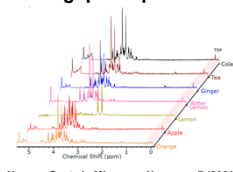
Sample preparation



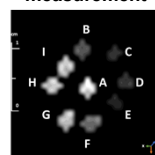
NMR measurement



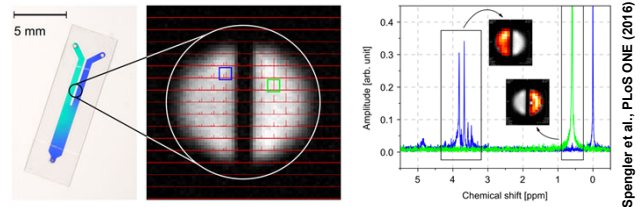
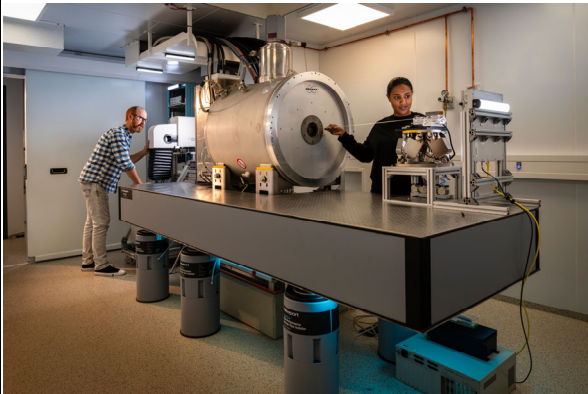
Throughput improved x50



Full titration, one measurement



CORREL lab @ IMT



Can we extract **more** information?

■ **Other** morphological/micro-structural features?

- porosity
- cracks
- sedimentation

5 November 20, 2023

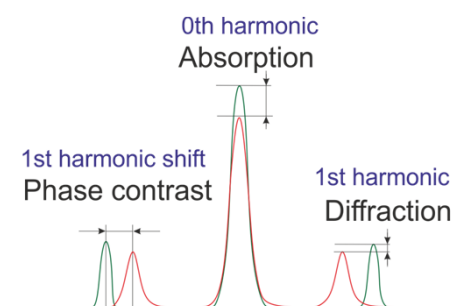
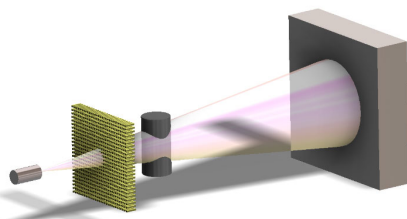
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X-ray imaging – **beyond absorption**



■ **Three** information channels

- absorption
- phase contrast
- diffraction



- high absorption-contrast materials
- internal borders – low absorption contrast
- scattering centres

6 November 20, 2023

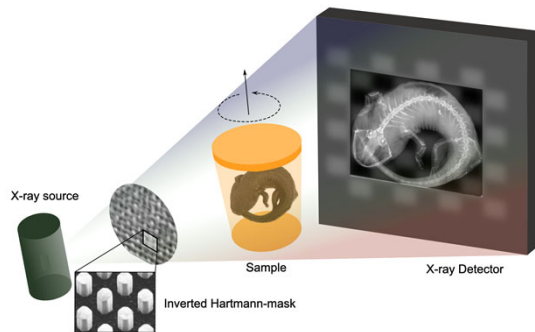
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Multimodal X-ray imaging for biological samples



- high absorption-contrast materials
- internal borders – low absorption contrast
- scattering centres

7 November 20, 2023

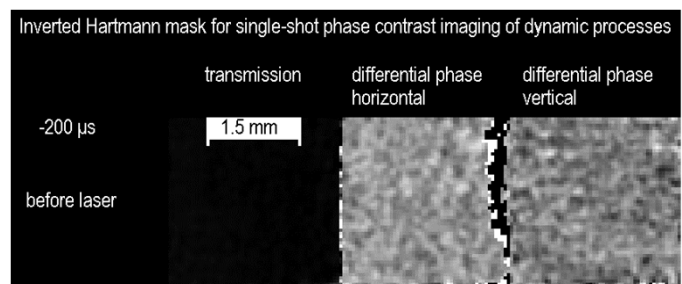
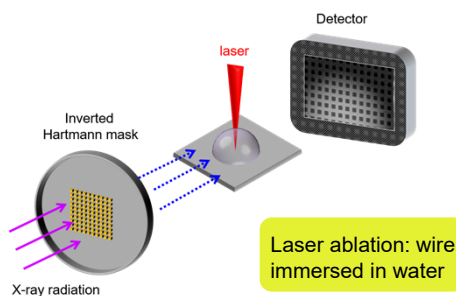
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Time-resolved X-ray imaging

- In-situ monitoring of dynamic processes



- Transmission information
- Differential phase information
 - horizontal
 - vertical

8 November 20, 2023

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Thank you!