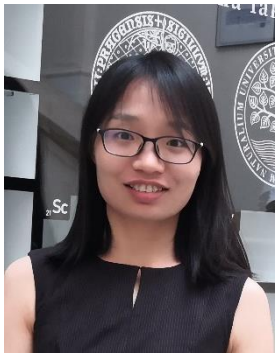
Department of Physical and Macromolecular Chemistry
invites you for a seminar
Lecture hall CH 3, Faculty of Science, Hlavova 8, Praha 2
on November 24th, 2021 at 14:00

NMR Simulation of Zeolites: An Approach combining *ab initio* Simulations and Machine Learning
speaker: Chen Lei

Finishing Ph.D. student, supervisor: Prof. RNDr. Petr Nachtigall, Ph.D.



Solid state ^{27}Al NMR (ssNMR) is an important technique to characterize the structure of catalytic sites in zeolites. To improve the interpretation of spectra, we developed a model based on DFT calculations to clarify the role of experimental conditions, lattice dynamic and local structure. We described the behaviour of a few zeolites accurately with the support of machine learning (ML), which can potentially simplify NMR calculation of zeolites.

Mechanochemistry for sustainable synthesis of framework materials
speaker: Daniel N. Rainer, M.Sc.

CUCAM; formerly: University of St.Andrews

Mechanochemical methods in synthesis chemistry help to alleviate concerns regarding sustainability, ecological considerations, and resource efficiency. Their success in the field of MOFs (metal-organic frameworks) has inspired us to investigate possibilities for production of sodium coordination polymers as well as zeolites with improved synthesis conditions compared to traditional routes.

Seminar will be available via Zoom: https://cuni-cz.zoom.us/j/94758328674
Organizers: Prof. Tomáš Obšil, Prof. Jiří Čejka, Dr. Jan Přech

Department of Physical
and Macromolecular Chemistry
Faculty of Science, Charles University,
Albertov 6, Prague 2
128 44, Czech Republic

Head of Department:
Prof. RNDr. Tomáš Obšil, Ph.D.
obsil@natur.cuni.cz
T: +420 221 951 289

IČO: 00216208
DIČ: CZ00216208