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Research in our theory group is devoted to modeling of realistic nanosystems in close collaboration with experimentalists. We use quantum and classical (atomistic and coarse-grained) molecular dynamics (MD) simulations, Monte Carlo and other techniques to model molecular and nanoparticle self-assembly, storage, transport, delivery, and (bio)-activity. We also study electronic structures and transport properties of complex nanosystems. The calculations are performed on our multiprocessor and GPU clusters and on national supercomputers.

Pozvánka na seminář

odd.

# MOLEKULÁRNÍ ELEKTROCHEMIE

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ELEKTROCHEMICKÝCH MATERIÁLŮ

v pátek 30.6. v 10:30 hod v zasedací místnosti 108

**Prof. Petr Král (University of Illinois at Chicago)**

**Modeling of Nanoparticles Self-assembly into Functional Superstructures**

First, we briefly discuss our pioneering studies of self-assembly and nanofluidics in graphitic systems [1]. Next, we present our recent hybrid modeling of nanoparticles formation and self-assembly in liquid cells, done in collaboration with experimentalists [2]. Then, we present atomistic molecular dynamics (MD) simulations [3] and mean-field Monte Carlo [4] modeling of nanoparticles self-assembly into chiral ribbons, magnetic helices, hollow shells, nanoreactors, and porous layers.

[1] K. Sint et al., JACS **130**, 16448 (2008); N. Patra et al., Nano Lett. **9**, 3766 (2009).

[2] N. Duane Loh et al., Nat. Chem. **9**, 77 (2017); G. Lin et al., ACS Nano **10**, 7443 (2016).

[3] J. Yeom et al., Nat. Mat. **14**, 66 (2015); H. Zhao et al., Nat. Nanotech. **11**, 82 (2016);

M. Yang et al., Nat. Chem. **9**, 287 (2016); T. Udayabhaskararao, *submitted*.

[4] G. Singh et al., Science **345**, 1149 (2014).

