

DEPARTMENT OF PHYSICS

**Chemical Physics Group**

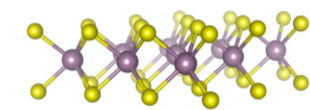
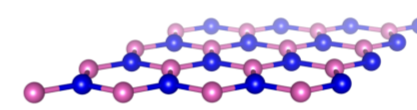
Wednesday, April 24th 2019, 2:00PM

Room L439, Chittussiho 10, Ostrava

**Group Seminar**

**14:00** František Karlický: Introduction

**Periodic systems and two-dimensional materials**



**14:05** Nikola Macháčová: Properties of graphene-based van der Waals heterostructures

**14:15** Miroslav Kolos: Many-body calculation of electronic and optical band gap of bulk hexagonal boron nitride

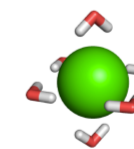
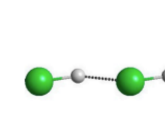
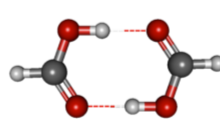
**14:30** Oto Kohulák: Polytypism in transition metal dichalcogenides

**14:45** Tomi Ketolainen: Optical gaps of two-dimensional materials by time-dependent density functional theory

**15:00** Luigi Cigarini: Stability of bulk hexagonal boron nitride

**15:15** Coffee break

**Molecular complexes and clusters**



**15:30** Martin Mrovec: An optimization approach to solving the Kohn-Sham equations

**15:45** Roman Fanta: Hydrogen bonds by fixed-node diffusion Monte Carlo

**16:00** Matúš Dubecký: Fractional charge by fixed-node diffusion Monte Carlo

**16:15** Michal Novotný: Absorption spectra of small mercury clusters: Equation-of-motion coupled-cluster method vs. time-dependent density functional theory

**16:30** René Kalus: Detection of phase changes in (mercury) clusters through their photoabsorption

**16:45** Discussion, closing