

Jakub Oprštný

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Education

2017-2020 **Bachelor**, VŠB - Technical University Ostrava, Nanotechnology.

Thesis: Phase stability of actinide carbides

Supervisor: Dr. Dominik Legut

Courses in mathematics, physics and chemistry, with focus on the study of structure and properties of nanomaterials, and their synthesis.

Experience

since 2019 **Research Assistant**, IT4Innovations National Supercomputing Center, Ostrava, Czech Republic.

Electronic Structure Group

Quantum mechanical calculations of electronic structure (such as density of states, bandgap), phase stability (both static and dynamic), elastic properties (elastic tensor and derivable elastic constants, elastic anisotropy), phonons at both harmonic and quasi-harmonic level and resulting thermal properties (phonon band structure and density of states, free energy, entropy, heat capacity at both constant volume and constant pressure, thermal expansion). Currently studying the phase stability and physical properties of U_2C_3 and Th_2C_3 .

Presentations & Publications

2019 5th workshop on ab initio phonon calculations, Cracow

Poster title: *Phase stability of Uranium and Thorium sesquicarbide*

Languages

Czech Native

English Proficient

Tools & Technologies

Linux, Windows

Bash, Python, C / C++

Matplotlib, Numpy, Scipy, MATLAB / Octave, Grace

VASP, Phonopy, AELAS, VASPKIT, p4vasp