SYLLABUS

1. Course title: **Molecular modeling in mineralogy**

2. Course lecturer: **dr hab. Marek Szczerba**

3. Field, type and level of studies, year of study: **geology, full-time doctoral studies, all years of study**

4. Course character: **elective** (see point B.1 in the *Curriculum of the full-time Doctoral Programme* – at least 4 ECTS points have to be gained during the studies)

5. Teaching method: **traditional** (personal contact with the lecturer) **and video conferencing**

6. Language: **Polish or English** (depending on the audience)

7. Course type and number of hours: **lecture (6 h), lab (4 h)**

8. Estimated amount of student's independent work: **10 h**

9. Total workload and number of ECTS points: **20 h, 1 ECTS**

10. Short description and main focus of the course:
    - introduction to molecular modeling,
    - interatomic potentials,
    - optimization methods, molecular mechanics,
    - programs for calculating and visualizing the results: LAMMPS and VMD,
    - Monte Carlo methods in molecular modeling, Towhee program,
    - results analysis, visualizations, TCL script language.

11. References:
    - Molecular Modelling for Beginners, Alan Hincliffe
    - https://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/
    - https://lammps.sandia.gov/doc/Manual.html
    - http://towhee.sourceforge.net/usersmanual.html

12. Educational outcomes:
    KNOWLEDGE: Has knowledge of the basics of molecular modeling / Knows and understands the basics of molecular modeling programs
    PRACTICAL SKILLS: Can use basic molecular modeling programs

13. Evaluation of the educational outcomes: **observation of student's commitment during the classes**

14. Criteria to complete the course: at least **80%** attendance, final grade depends on the evaluation of the student's commitment during the classes.