



MATERIALS SCIENCE AND SIMULATION Summer 2016

## INTERFACES AND SURFACES

Mon 10:15 and Thu 12:15 in IC 02/718 or the ICAMS CIP-pool IC 02/522

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Surfaces and interfaces influence optical, electronic, and mechanical properties of materials. Thus they play an important role in many areas of material science, such as semiconductor technology, the development of new structural materials, or the field of catalysis.

To obtain a fundamental understanding of processes taking place at surfaces and interfaces, investigations on a microscopic level are necessary. It is nowadays possible to study interfaces and surfaces with atomic resolution both experimentally and theoretically.

In this course, we will give an overview of the relevance of surfaces and interfaces in materials science and the experimental and computational techniques to characterise them. We will discuss the relationship between the atomistic description of interfaces and surfaces, and the resulting macroscopic materials properties, especially electronic and mechanical properties.

The lectures will be complemented by exercises as well as hands-on classes on computational techniques. The course is intended for M. Sc. students. Successful completion including a written exam will correspond to 6 credit points.

### Keywords:

- interface/surface crystallography, relaxation/reconstruction
- adsorbates, defects, vacancies, impurities
- interface characterisation: diffraction, scanning, microscopy, and spectroscopy
- thermodynamics and mechanics of interfaces
- modeling: empirical concepts, electronic structure, atomistic simulation

### Literature:

- A. Gross, Theoretical Surface Science: A Microscopic Perspective
- F. Bechstedt, Principles of Surface Physics
- J.M. Howe, Interfaces in materials

### First lecture:

Monday, April 11, 2016 at 10:15 a.m. in IC 02/718

If you have further questions, please get in touch with [Rebecca.Janisch@rub.de](mailto:Rebecca.Janisch@rub.de), [Jutta.Rogal@rub.de](mailto:Jutta.Rogal@rub.de) or [Thomas.Hammerschmidt@rub.de](mailto:Thomas.Hammerschmidt@rub.de).