**Atomistic and quantum simulations of materials**

**Cursus**

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<th>Science et génie des matériaux</th>
<th>Sem.</th>
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**Language** English

**Credits** 4

**Session** Summer

**Semester** Spring

**Exam** During the semester

**Workload** 120h

**Weeks** 14

**Hours** 120h

4 weekly

2 weekly

**Lecture**

2 weekly

**Practical work**

2 weekly

**Number of positions**

**Remarque**

pas donné en 2018-19

**Summary**

Theory and application of quantum simulations to model, understand, and predict the properties of real materials.

**Content**


**Learning Prerequisites**

**Recommended courses**

Fundamentals of solid-state materials, or similar.

**Learning Outcomes**

By the end of the course, the student must be able to:

- Model materials with quantum mechanical simulations

**Teaching methods**

Ex cathedra and computational laboratories

**Assessment methods**

Written reports of computational labs