Universität Stuttgart

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Master Materials Science
Winter Semester 2021/22

„Advanced Science Seminar“

— *Ab initio*, machine learning, molecular dynamics —

You can choose one among the following topics:

1. ***Ab initio* simulations for Li-battery related materials**
   - ⇒ ACS Applied Materials & Interfaces 9 (2017) 40197–40206
   - ⇒ Chemistry of Materials 30 (2018) 5516–5517
2. ***Ab initio* simulations for perovskite oxides**
   - ⇒ Inorganic Chemistry 60 (2021) 10923−10933
   - ⇒ Chemistry—A European Journal 27 (2021) 1-6
3. ***Ab initio*-based diffusion simulations**
   - ⇒ Journal of Phase Equilibria and Diffusion 37 (2016) 44–52
   - ⇒ Physical Review Materials 3 (2019) 095601
4. ***Ab initio* thermodynamic properties**
   - ⇒ Physical Review B 91 (2015) 214311
   - ⇒ Physical Review Letters 114 (2015) 195901
5. **Machine learning, specifically Moment Tensor Potentials**
   - ⇒ Physical Review Materials 5 (2021) 073801
   - ⇒ Machine Learning: Science and Technology 2 (2021) 025002
6. **Molecular dynamics of NiTi shape memory alloys**
   - ⇒ Acta Materialia 123 (2017) 90-101
   - ⇒ PhD thesis on NiTi

Since it is likely that the topics will not tell you much at this stage, you can use the given references (hyperlinked) to get some first insights. More literature can be provided to you once you decide for a topic, but you are encouraged to search through the relevant scientific papers yourself.

The procedure is then as follows:

1. You choose the topic and fix your choice in the following doodle survey. Be quick, first come, first serve.

   doodle.com/poll/22ipfn8kcn57x2ym?utm_source=poll&utm_medium=link

2. You join the kick-off meeting on **27th October 2021** starting at **9 am**. This initial meeting will be held online in my WebEx room: https://unistuttgart.webex.com/meet/blazej.grabowski
3. In the kick-off meeting we will assign the seminar dates to every student. The possible dates will be on **Wednesdays from 9 am to 12 am** later in the semester so that you have enough time for preparation.
4. You work yourself into the topic by studying the literature. Additionally, you will have an experienced researcher as a contact person to ask questions. You need to meet with your contact person at least once prior to your seminar to discuss your progress and the presentation.
5. You give your presentation (about 30 min + additional time for discussion) in a seminar style to the other students. The seminar will take place **in presence** (3G rules apply) in a seminar room (to be announced) in the chemistry building (Pfaffenwaldring 55). You also need to attend the other student's presentations and be active in discussions.

That's about it. After successfully finishing point 5, you have passed the Advanced Science Seminar.

With best regards,

Prof. Dr. Blazej Grabowski