

Invitation to workshop
„Computational Methods for Periodic Systems“
08. - 09. July 2013

The aim of this small, local workshop is to

- Provide basic knowledge of quantum chemistry computer codes (VASP, ADF-BAND, SIESTA) for periodic systems. Additionally, one GAUSSIAN session will cover molecular calculations.
- Give an overview of the capabilities of these codes for computation of properties
- Enable exchange of know-how for researchers familiar with the codes

The previous workshop was well received:

http://www.uni-marburg.de/fb15/ag-tonner/events/event001?set_language=en

We will have Dr. Daniel Sanchez-Portal from San Sebastian as external guest.

Apart from that, the Tonner group will give presentations on relevant topics.

The workshop has a rather informal character and will take place in a relaxed atmosphere to enable mutual exchange of ideas and knowledge.

The workshop is jointly organized with and kindly supported by the GRK 1782 „Functionalization of semiconductors“.

The workshop takes place:

Monday and Tuesday until 2 pm

in the Schulungsraum of the Hochschulrechenzentrum Marburg. Room 06A07, Mehrzweckgebäude, Lahnberge.

Tuesday 2 pm – 4 pm

Seminar room E4 /4326 in the Fachbereich Chemie.

Please register via the following Doodle list until Wednesday, 03.07.2012:

<http://doodle.com/sgeinbm35ivpsmgw>

Tentative Schedule

Day 1	Program
9.45 – 10.00	Arrival
10.00 – 11.30	„An introduction to periodic calculations – example VASP“ (Ralf Tonner)
11.30 – 12.00	Hand-On VASP
<i>12.00 – 13.00</i>	<i>Lunch break</i>
13.00 – 14.00	„The SIESTA code“ (Daniel Sanchez-Portal)
14.00 – 15.00	Hands-On SIESTA
<i>15.00 – 15.30</i>	<i>Coffee break</i>
15.30 – 16.00	„GAUSSIAN09 – basics of molecular calculations“ (Andreas Stegmüller)
16.00 – 16.30	Hands-On GAUSSIAN09
16.30 – 17.00	„ADF-BAND – chemical bonding in periodic systems“ (Marc Raupach)
17.00 – 17.30	Hands-On ADF-BAND
<i>Evening</i>	<i>Drinks downtown</i>

Day 2	
10.00 – 11.00	„Electronic structure, properties and phonons with VASP“ (Phil Rosenow, Ralf Tonner)
11.00 – 11.45	Hand-On VASP
12.00 – 13.00	Visualisation options, Scripting, Tools (AG Tonner)
<i>13.00 – 14.00</i>	<i>Lunch break</i>
14.15 – 15.00	„GW methods in SIESTA“ (Daniel Sanchez-Portal)
15.00 – 16.00	Further selected topics (AG Tonner)
