

Report on NOMAD Summer, a Hands-on Course on Tools for Novel Materials Discovery

The first NOMAD (**N**ovel **M**aterials **D**iscovery) summer school, called *NOMAD Summer*, a Hands-on Course on Tools for Novel Materials Discovery was held from September 25 - 29, 2017, in Berlin,

Germany. Being fully dedicated to data-driven research, it was the first of this kind world-wide and as such got a lot of attention.

In order to support our participants in an optimal way, providing computer equipment for everyone, we had to restrict their number to 40. These 40 attendees reflected the broad audience that NOMAD addresses, covering students, academic researchers as well as representatives of small and large research labs and enterprises.

This workshop did not only demonstrate NOMAD's achievements, but also taught the usage of the wide range of NOMAD tools, in order to take advantage of these developments and the large amount of data gathered by this project. The eight sessions were organized by topics, covering

- Data repositories
- NOMAD Encyclopedia
- Advanced Graphics
- High-throughput calculations & data quality
- Data analytics (four sessions)

Each of the sessions started with talks, giving scientific insight and preparing the ground for the following hands-on sessions. The availability of on-site computing resources and many tutors ensured the best possible assistance for the attendees. The easy handling of the NOMAD tools was also strongly enhanced by relying on NOMAD's concept for its infrastructure, which neither needs any installations or preparations on the clients' computers, nor any other (even user-friendly) state of the art tool (like e.g. Jupyter notebooks).

The program was complemented by keynote talks by (external) speakers, S. Curtarolo (Duke University), D. Kranzlmüller (LRZ Munich, now NOMAD PI), A. von Lilienfeld (University of Basel), T. Mueller (Johns Hopkins University), G. Paliana (Los Alamos National Laboratory), and J. Vybiral (Charles University Prague). Delightful talks about how visualization can help with scientific insight, and about how to design an application from a user-experience expert point of view shed light on the possible ways of presenting and transferring knowledge.

The sessions on *Data repositories* and the *NOMAD Encyclopedia* demonstrated how to access the computational materials science data, as stored and processed by NOMAD, via graphical interfaces and APIs. The session on *Visualization* amazed the audience with the possibilities of using virtual reality tools on commodity devices like mobile phones as well as specialized equipment.

High throughput calculations and data quality drew very strong attention by the industrial sector.



The scientifically exciting progress in a whole range of applications of data-analytics was emphasized in four sessions on different topics, i.e., *Structure prediction*, *Cluster expansion & thermodynamics*, *Materials' properties prediction*, and *Kernel methods*.

Another integral aspect of the school was to bring together students, experienced academics, and industry representatives with the NOMAD team. To foster the exchange between the communities, we organized an excursions to Teufelsberg, a former US listening station, with 120m above sea level the highest point in the Berlin area.

The feedback from attendees as well as lecturers was extremely positive. We even received some very nice comments afterwards as, for example an industry representative recognized that his recommendations had been implemented in the Encyclopedia. The NOMAD Encyclopedia statistics also show a persistent increase of usage since the event.

The full program as well as videos of the talks and tutorial material can be found at the event's homepage <http://meetings.nomad-coe.eu/nomad-summer-2017/>.

The second edition of *NOMAD Summer* will be held from September 24 – 27, 2018, in Lausanne, Switzerland, see <http://meetings.nomad-coe.eu/nomad-summer-2018/>.

	First Name	Name	Affiliation
1	Jan	Vybiral	Charles University Prague
2	Ghanshyam	Pilania	Los Alamos National Laboratory
3	Tim	Mueller	Johns Hopkins University
4	Anatole	von Lilienfeld	University of Basel
5	Stefano	Curtarolo	Duke University
6	Dieter	Kranzlmüller	LRZ München
7	Matthias	Scheffler	Fritz-Haber-Institut
8	Angelo	Ziletti	Fritz-Haber-Institut
9	Emre	Ahmetcik	Fritz-Haber-Institut
10	Mario	Boley	MPG Saarbrücken
11	Luca	Ghiringhelli	Fritz-Haber-Institut
12	Runhai	Ouyang	Fritz-Haber-Institut
13	Xiangyue	Liu	Fritz-Haber-Institut
14	Daria	Tomecka	Fritz-Haber-Institut
15	Christian	Carbogno	Fritz-Haber-Institut
16	Fawzi	Mohamed	Fritz-Haber-Institut
17	Alfonso	Sastre	Fritz-Haber-Institut
18	Claudia	Draxl	Humboldt-Universität zu Berlin
19	Pavone	Pasquale	Humboldt-Universität zu Berlin
20	Fu	Qiang	Humboldt-Universität zu Berlin
21	Caruso	Fabio	Humboldt-Universität zu Berlin
22	Jungho	Shin	Humboldt-Universität zu Berlin
23	Lorenzo	Pardini	Humboldt-Universität zu Berlin
24	Santiago	Rigamonti	Humboldt-Universität zu Berlin
25	Luz	Calvo	Barcelona supercomputing Center
26	Georg	Huhs	Barcelona supercomputing Center
27	Kristian	Thygesen	DTU
28	Martina	Stella	King's College
29	Adam	Fekete	King's College
30	Ruben	Garcia Hernandez	LRZ
31	Markus	Rampp	MPDCF
32	Michele	Compostella	MPDCF
33	Mikkel	Strange	DTU
34	James	Kermode	University of Cambridge
35	Gabor	Csanyi	University of Cambridge
36	Sabrina	Sicolo	BASF SE
37	Daria	Galimberti	Universite d'Evry val d'Essonne
38	Jin Hyun	Chang	Technical University of Denmark
39	Alvaro	Cimas	Université d'Evry val d'Essonne
40	Daniel	Urban	Fraunhofer IWM
41	Wolfgang	Mannstadt	Schott AG

42	Kerstin	Hummer	University of Vienna
43	Simon	Loftager	Technical University of Denmark
44	Michael	Rieger	BASF SE
45	Azimatu	Seidu	Aalto University
46	Martin	Friak	Institute of Physics of Materials, Czech Academy of Sciences
47	Caetano	Rodrigues Miranda	University of Sao Paulo
48	Carina	Arasa Cid	Elsevier
49	Kisung	Chae	Korea Institute for Advanced Study
50	Ansgar	Schäfer	BASF SE
51	Berk	Onat	University of Warwick
52	Anuradha	Ashok	Shell Technology Centre
53	Yu-Chieh	Lin	Materials and Chemical Research Laboratories
54	Che-Ming	Chang	Industrial Technology Research Institute
55	Béla	Fiser	University of Miskolc
56	Mathias	Augustin	Queen's University of Belfast
57	Steen	Lysgaard	Technical University of Denmark
58	Estefanía	Garijo del Río	Technical University of Denmark
59	Anders	Riis-Jensen	Technical University of Denmark
60	Pascal	Boulet	Aix-Marseille University
61	Guohua	Cao	Wuhan University
62	Mario	Burbano	Maison de la Simulation
63	Guangzhao	Qin	RWTH Aachen University
64	Ayana	Ghosh	University of Connecticut
65	Deepak	Jain	Tata Consultancy Services Limited
66	Roman	Schmack	TU Berlin
67	Andris	Gulans	HU Berlin
68	Markus	Scheidgen	HU Berlin
69	Saeideh	Edalati Boostan	Giessen
70	Alexandra	Toumar	ICMCB-CNRS
71	Ivan	Marri	Istituto Nanoscienze S3 CNR

Teilnehmer Dokdoranden/Masterstudenten

72	Maria	Troppenz	Humboldt-Universität zu Berlin
73	Axel	Hübner	Humboldt-Universität zu Berlin
74	Benedikt	Hoock	Humboldt-Universität zu Berlin
75	Martin	Kuban	HU Berlin
76	Phil	Preikschas	TU Berlin
77	Dennis	Trujillo	University of Connecticut
78	Andreas	Jeindl	University of Technology Graz
79	Sebastian	Tillack	Humboldt-Universität zu Berlin