



NOMAD

NOVEL MATERIALS DISCOVERY



Novel Materials Discovery: NOMAD

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Leibniz Supercomputing Centre,
Bavarian Academy of Sciences

Dissemination Session

PRACE-CoEs-FETHPC-EXDCI Workshop

Brühl, Germany. 30 October 2018

Who I am

What I work on

NOVEL MATERIALS DISCOVERY

- Rubén García - Specialization in Virtual Reality
Deputy PI of NOMAD Advanced Graphics
- NOMAD Repository: largest collection of materials science simulations
- Code-independent view (archive)
- Material-centric property view (encyclopedia)
- Machine learning to discover new properties and descriptors (big-data analytics)
- Advanced graphics for interactive data exploration



THE ARCHIVE



NOMAD
REPOSITORY



MATERIALS
ENCYCLOPEDIA



ADVANCED
GRAPHICS



BIG-DATA
ANALYTICS



OUTREACH



HPC
INFRASTRUCTURE

Dissemination activities that worked well

NOVEL MATERIALS DISCOVERY

- Summer of Simulation 2017 at the Leibniz Supercomputing Centre of the Bavarian Academy of Sciences (25 October 2017)
- Increased awareness of NOMAD VR at LRZ
- NOMAD VR is used at Technical University of Munich Theoretical Chemistry Chair
- NOMAD VR also used to visualize Fluid Dynamics at TUM.



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Dissemination activities that did not work well and why

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- WATOC 2017. 11th Triennial Congress of the World Association of Theoretical and Computational Chemists. Virtual-reality view on chemistry and materials science. Rubén Jesús García-Hernández, Claudia Draxl, Matthias Scheffler and Dieter Kranzlmüller. Poster Session 3, pp 299
- Lots of interest in testing the VR setup
- However, no follow-up communications



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Dissemination activities in preparation

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- Talk at the LRZ Extreme Scaling Workshop
- Early 2019, 3 day event
- Presentations regarding SuperMUC NG

- 30 minute talk with NOMAD and NOMAD VR overview.



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