NOVEL MATERIALS DISCOVERY

Creation of 360° videos from volumetric datasets

Use cases: Excitons in lithium fluoride

Adsorption of carbon dioxide on calcium oxide

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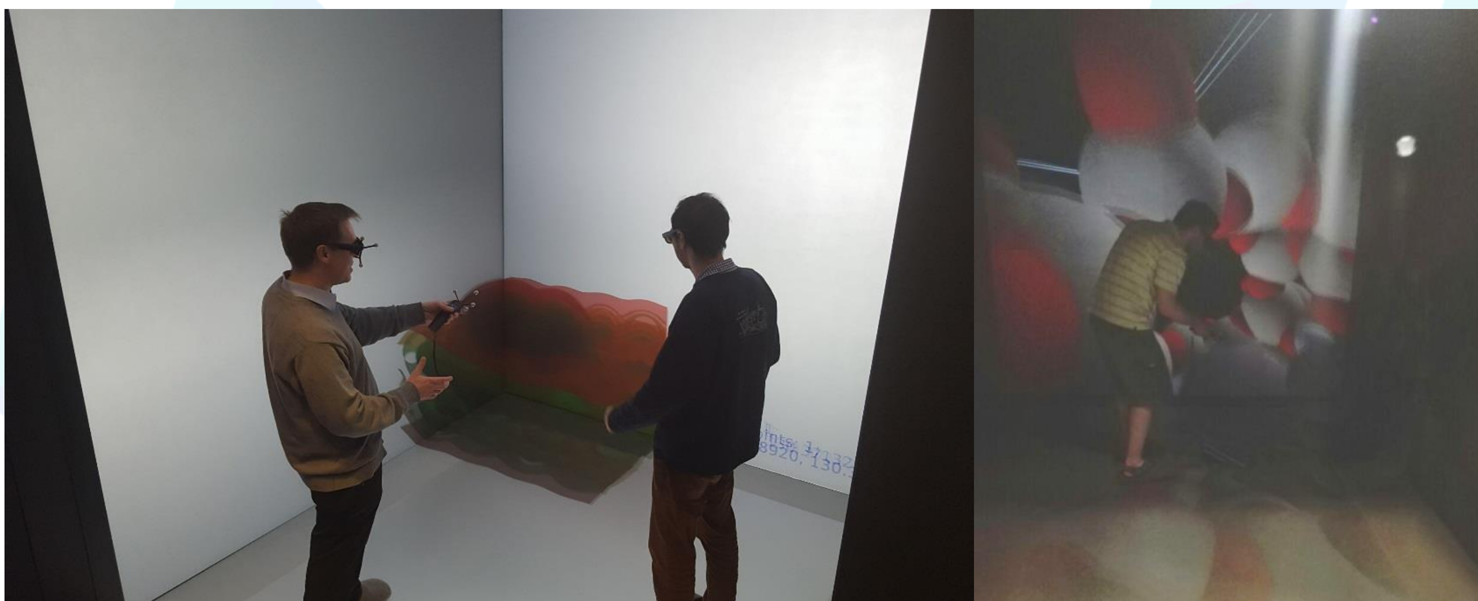
SuperMUC Status and Results Workshop 2018
Garching, Germany. July 25, 2018

Field: Materials Science

Exploring chemical reactions to discover optimal materials for given usecases and new properties of existing materials



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NOMAD Overview

- 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
- VR technology allows a view into the nanoscale

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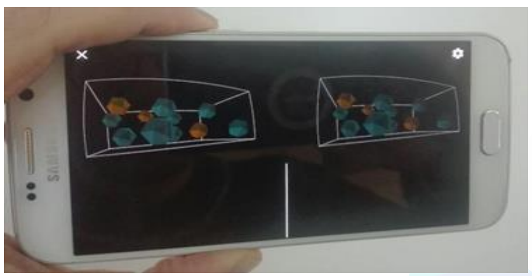
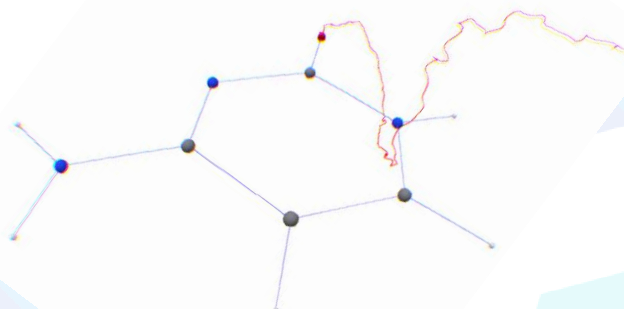
Virtual Reality: General viewer

Crystal structures, integrated with encyclopedia



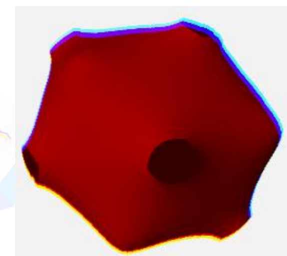
Nb_8As_4 (space group 62)

Molecular dynamics



Cytosine

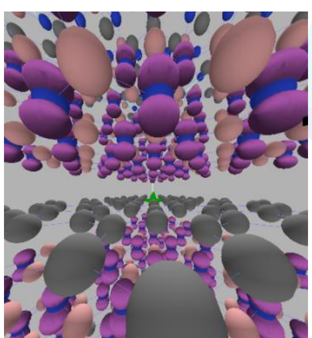
Fermi surfaces



Ag

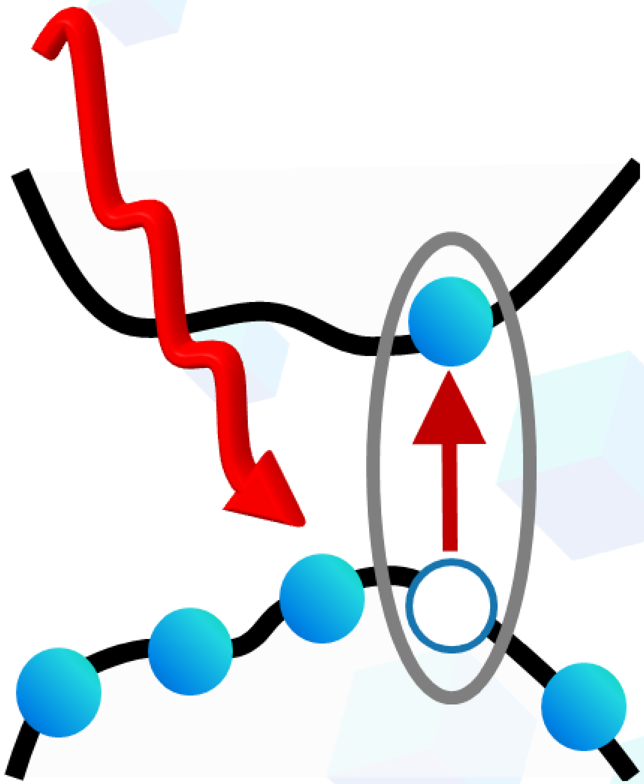
Electron density

CO_2-CaO adsorption



Excitons, graphene-BN heterostructures

Excitons: electron-hole pairs

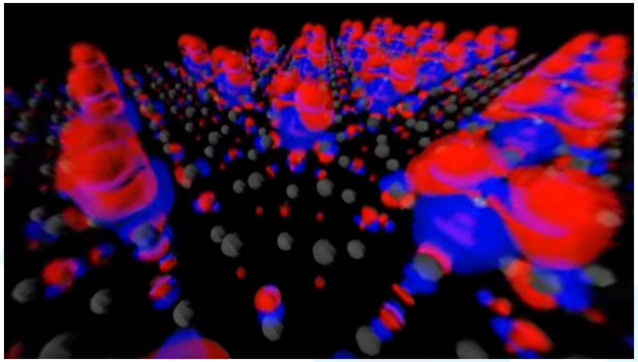


$$\phi_\lambda(\mathbf{r}_e, \mathbf{r}_h) = \sum_{cv} A_\lambda^{cv} \psi_c(\mathbf{r}_e)\ \psi_v(\mathbf{r}_h)$$

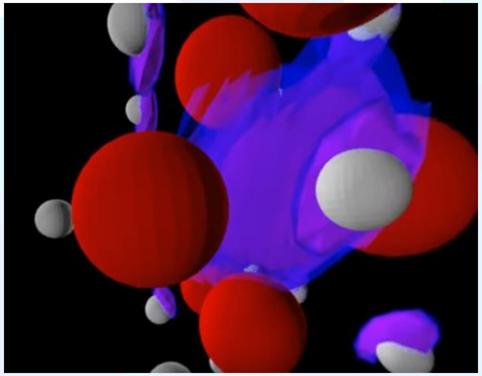
$$\phi_\lambda(\mathbf{r}_e, \mathbf{r}_h)$$

Example datasets for Outreach: video creation

- Two example chemical systems chosen:
  - Adsorption of CO_2 on CaO surface
    - 4D dataset, time evolution of electron density
      https://youtu.be/zHlS_8PwYYs



  - Electron-hole (exciton) interaction in LiF
    - 6D dataset
      https://youtu.be/XPPDeeP1coM



- Use of the pipeline for virtual reality preprocessing to generate stereo, panoramic videos

Immersive, 360° video creation

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- We use Blender with the cycles renderer, which has support for creation of 360° panoramas
- Isosurfaces (ply) can be imported directly
- Atoms in xyz format can be imported by using an external plugin https://wiki.blender.org/index.php/Extensions:2.6/Py/Scripts/Import-Export/XYZ (alternative, export to vrml using paraview or other software)
- Python scripting can be used to load the scene, setup the camera and render frames
- Use e.g. ffmpeg to prepare the video

ParaView FFmpeg

Immersive, 360° video creation

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Things to take into account:

- Cycles is physically based -> new material definitions
- High resolution required: 8k or 16k
  - 8k for visualization in VR devices
  - 16k for upload to youtube, because of the zoom control
  - This means: high memory and cpu requirements for video generation
- High quality rendering in the raytracing parameters to avoid flickering (samples per pixel)

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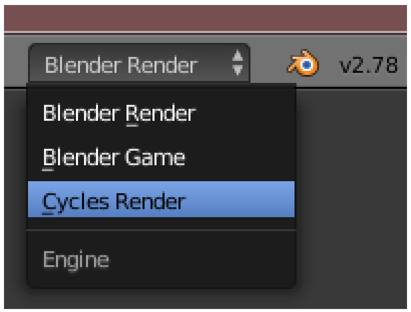
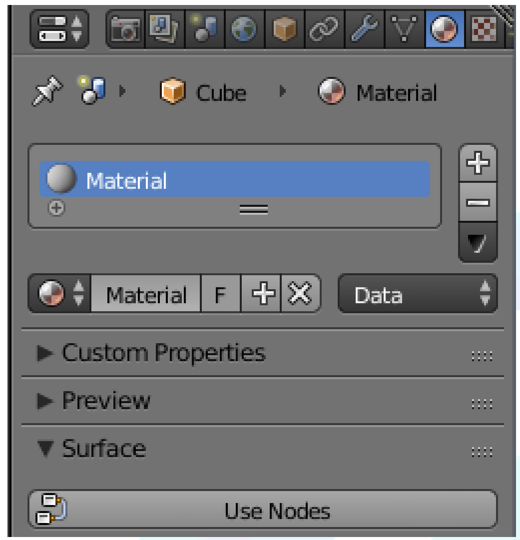
Immersive, 360° video creation

Example

Enabling Cycles



Use Nodes for physically based BRDF



Change the camera Lens to Panoramic

Type: Equirectangular

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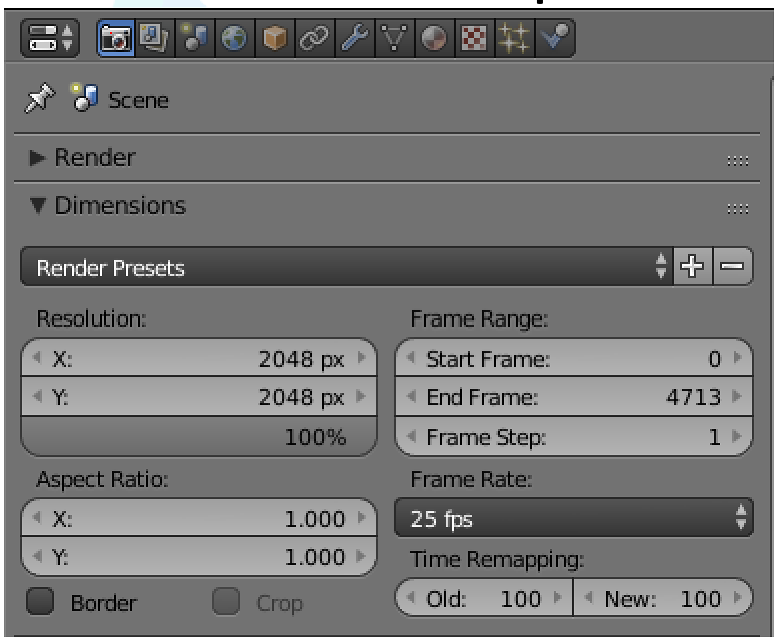
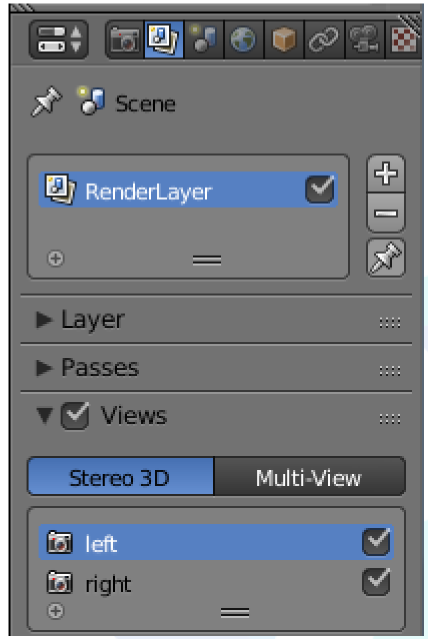
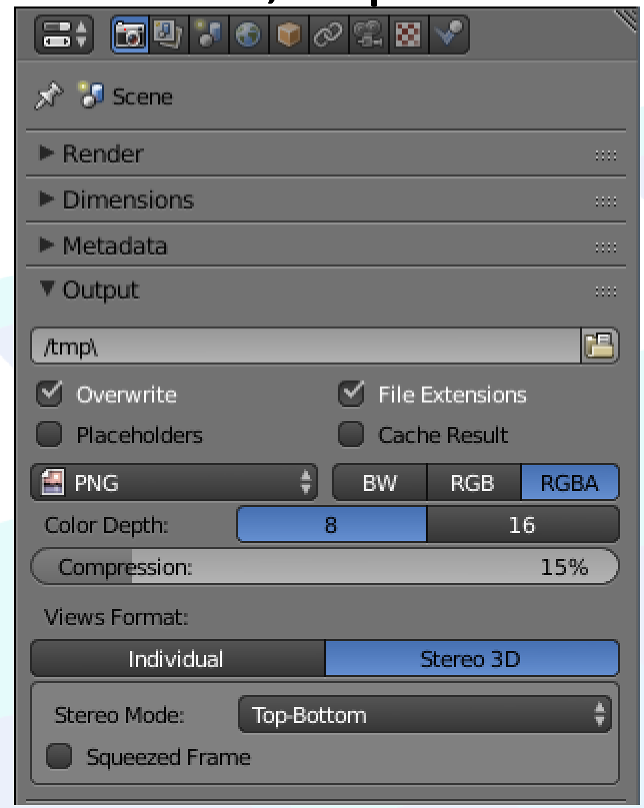
Resolution and aspect ratio



Stereo



Stereo3D, top-bottom



Raytracer

Samples

Highlights of the Python scripts

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Loading, cloning, transform, render, save

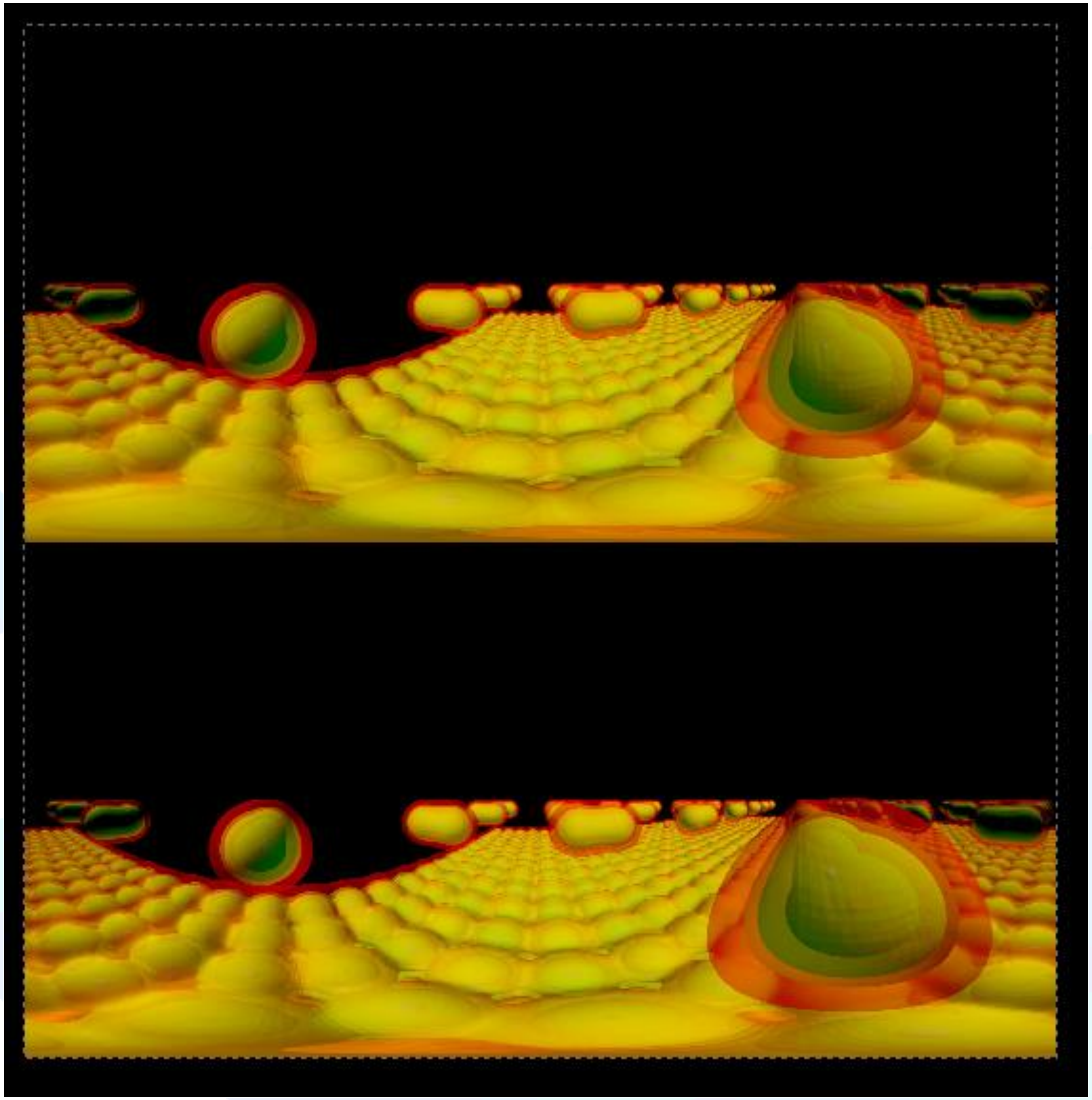
```
import bpy
matISO1=bpy.data.materials.get("ISO0001")
        # loop through frames
camera.location=(…)
bpy.ops.import_mesh.ply(filepath=string)
bpy.context.scene.objects.active.data.materials.append(mat)
M=bpy.data.objects.new("atom %d %d" %(i,j), MBase.data.copy())
scn.objects.link(M); scn.update()
M.location=…; M.scale=…; M.parent=…;
bpy.data.scenes["Scene"].render.filepath=OUTPUTPATH % time
bpy.ops.render.render(write_still=True )
```

Cleanup

```
for o in bpy.data.objects:
   if (o.type=='MESH'):
      scn.objects.unlink(o)
      o.user_clear()
      bpy.data.objects.
                 remove(o)
```

Immersive, 360° video creation

Resulting frame:



Immersive, 360° video creation

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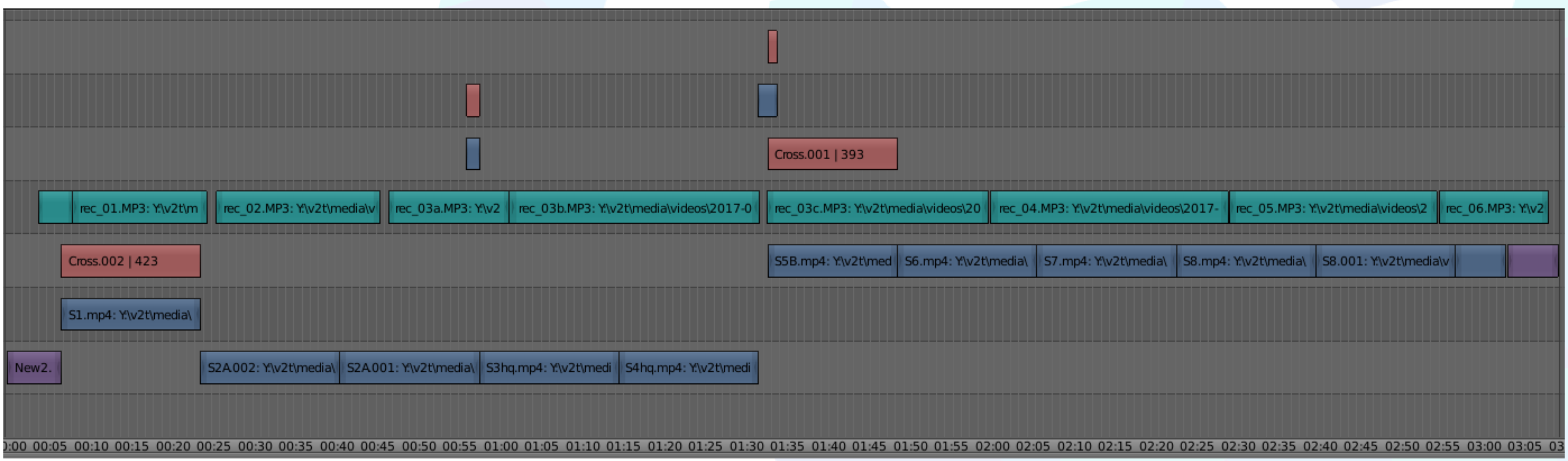
Various scenes and audio tracks can be combined to create the final video

Video-editing panel of Blender



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Rendering in SuperMUC

- Raytracing is an expensive algorithm, especially at the resolutions and quality settings required for 360° video
- Each frame can be calculated independently, so parallel batch jobs can be used to calculate multiple frames simultaneously.
- Since each frame may take a different time, CPU use is maximized by calculating various consecutive frames in each blender instance
- Cycles was added in a relatively recent version of blender, so proot can be used to run the newest version within a suitable environment

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SuperMUC resources used

- LRZ Linux Cluster and SuperMUC were used to render parts of the movies.
- Each frame takes about 7 hours of wall processing time on the 24 core machines (i.e. 168 CPU hours / frame).
- 941 frames rendered.
- Total = 158088 CPU-hours

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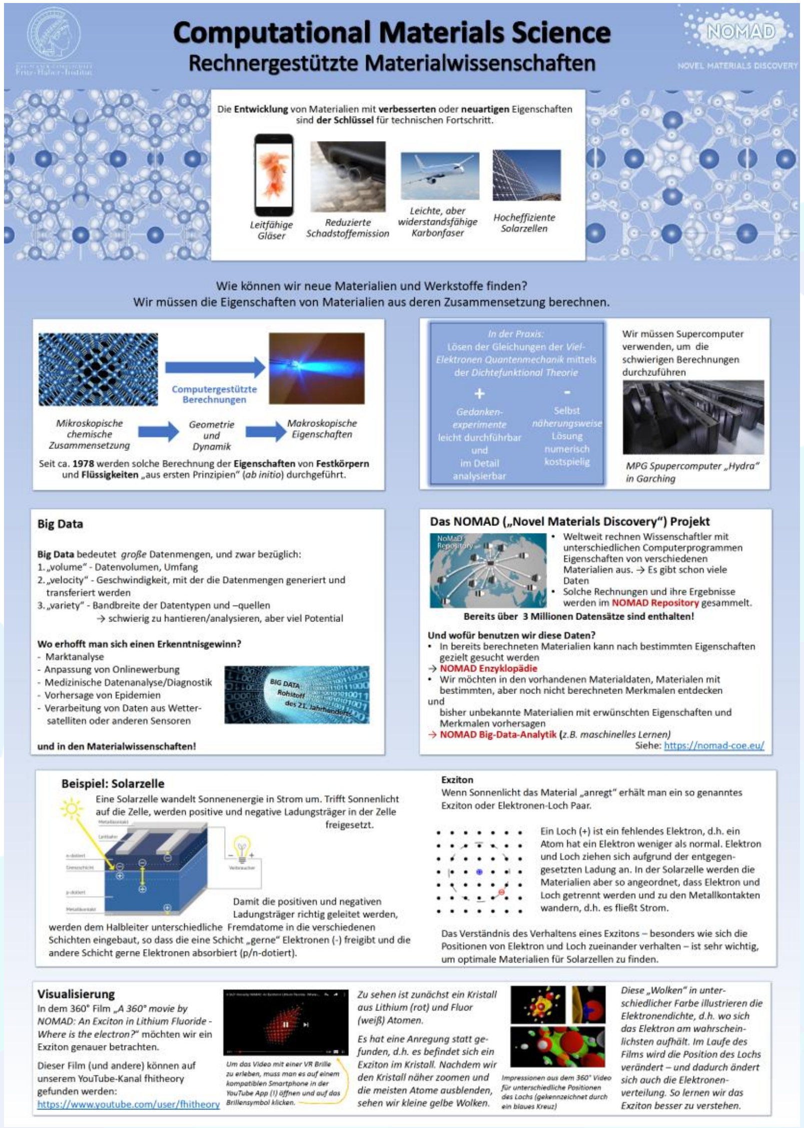
Example usecase: Long Night of Science

- Immersive exciton visualization
- Showcased during the Long Night of Science in Berlin, at the Fritz-Haber-Institut der Max-Planck-Gesellschaft
- Youtube + Google Cardboard
- A 360° movie by NOMAD: An Exciton in Lithium Fluoride – Where is the electron?



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V2C
VR and Visualisation Centre

lrz

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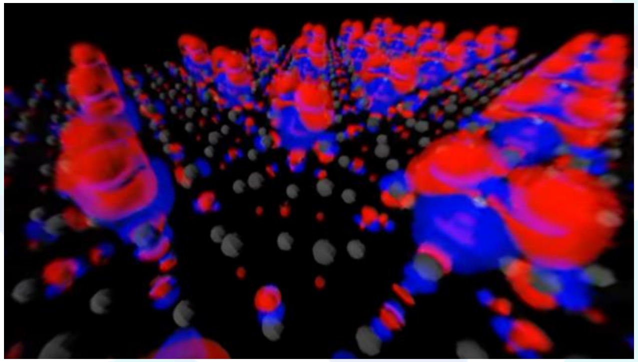
360° Video Demo & Questions

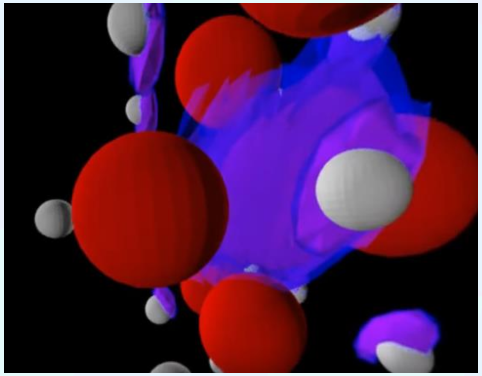
Adsorption of CO_2 on CaO surface

https://youtu.be/zHlS_8PwYYs



Electron-hole (exciton) interaction in LiF

https://youtu.be/XPPDeeP1coM



Extra Slides

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Stereoscopic video creation

(Stereoscopic) video creation

- The HTC Vive allows creation of monoscopic or stereoscopic videos.
- Procedure:
  - Indicate in the config file if monoscopic or stereoscopic is desired
  - Press the menu button to start/stop the recording of screenshots
  - Use e.g. ffmpeg to prepare the video

(Stereoscopic) video creation

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- The NOMAD Remote Visualization can also be used to create stereoscopic videos.
- Procedure:
  - Create the scene you want to display using VisIt GUI/CLI
  - Select the "Stereo" option in the "Set save options" →"Format options" tab. This will render each scene twice: once for the left eye, one for the right eye.
  - Merge each set of frames individually, creating 2 movies, one for each eye.
  - Arrange the movies in a side-by-side frame for visualization by stereoscopic-enabled devices.

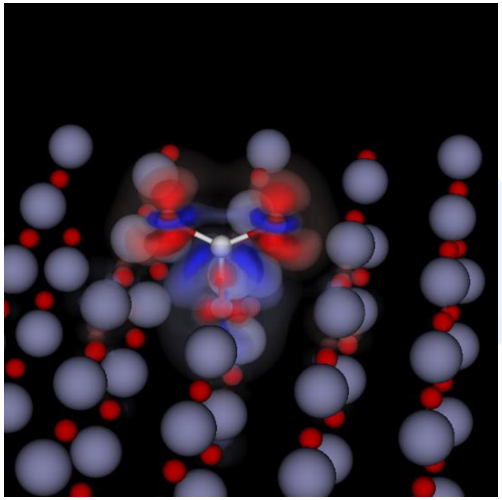
(Stereoscopic) video creation

- Examples (MPCDF, HUB):

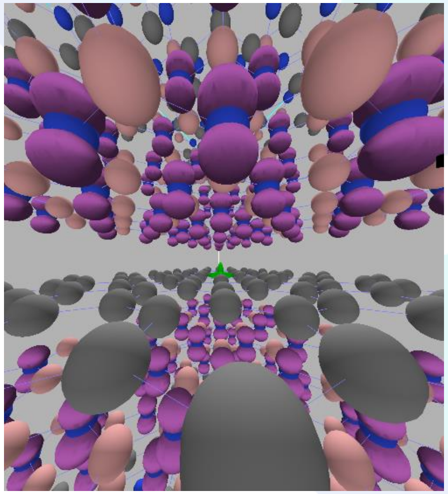
https://youtu.be/1ytS7n2IIqw
https://www.youtube.com/watch?v=tQrAPuFpFh8

https://www.youtube.com/watch?v=2c0mQp6RYXA

CO_2@CaO adsorption



graphene/BN heterostructure excitons



pyridine@zinc oxide