

Virtual Reality toolset for Material Science: NOMAD VR tools

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Virtual Reality toolset for Material Science: NOMAD VR tools

- NOMAD
- Chemical systems
- Developed VR tools
- Supported Hardware
- User Study
- Future work
- GearVR Demo and Questions

NOMAD

- Center of Excellence in Material Science
- Includes
 - Repository
 - Archive
 - Encyclopedia
 - Big Data analytics
 - Advanced Graphics
 - Infrastructure

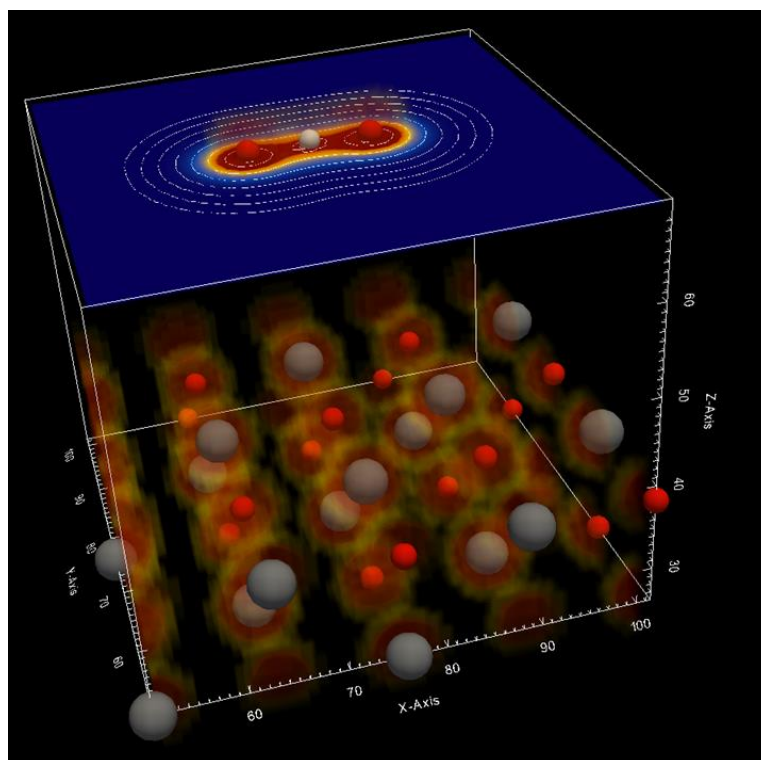


Example datasets

- Two example chemical systems were chosen within the NOMAD dataset for this prototype proof of concept
 - Adsorption of CO_2 on CaO surface
 - 4D dataset, time evolution of electron density
 - Electron-hole interaction in LiF
 - 6D dataset, due to quantum effects

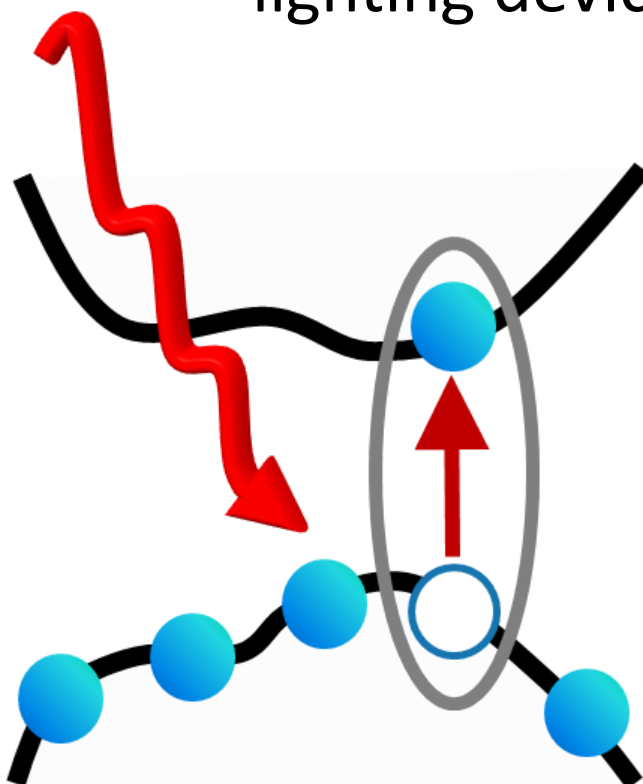
Adsorption of CO₂ on CaO surface

Relevant for carbon dioxide capture, activation and further transformation into other materials useful for industry.



LiF excitons

Excitons: Relevant in opto-electronics, solar cells, lighting devices, photocathalysis, water splitting

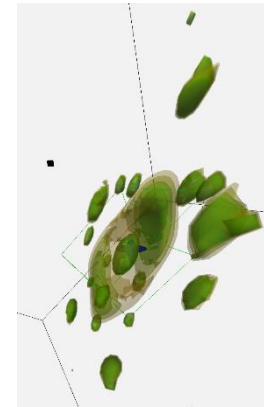
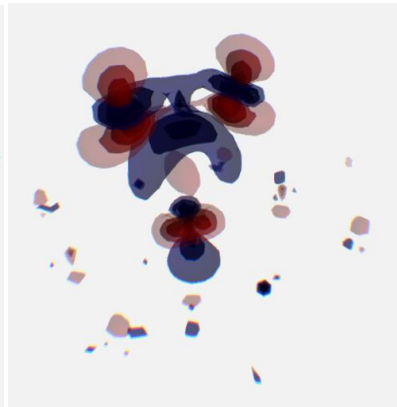
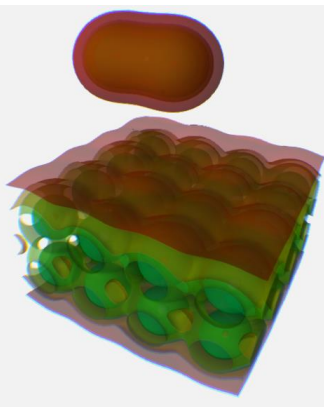
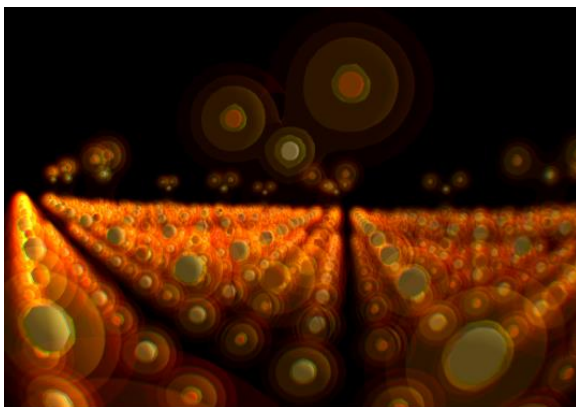


$$\phi_{\lambda}(\mathbf{r}_e, \mathbf{r}_h) = \sum_{cv} A_{\lambda}^{cv} \psi_c(\mathbf{r}_e) \psi_v(\mathbf{r}_h)$$

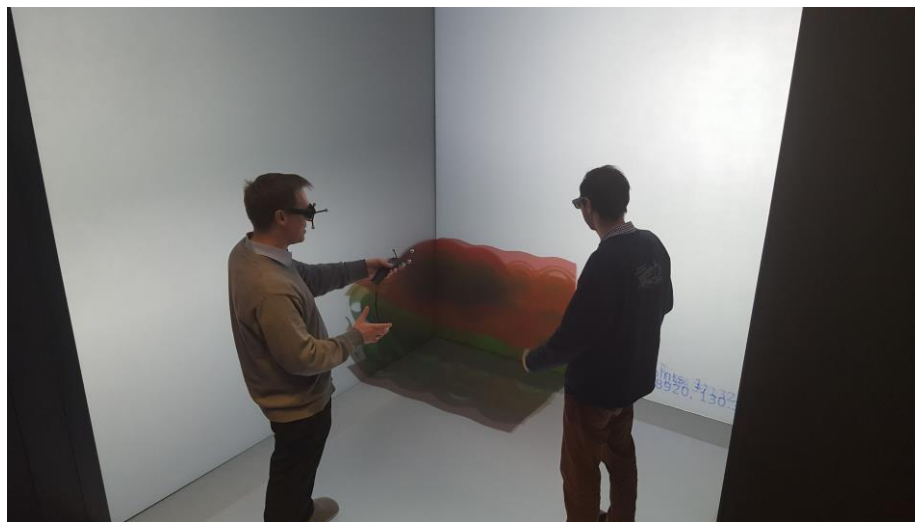
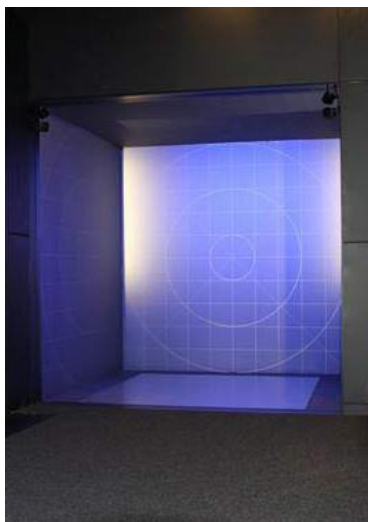
$$\phi_{\lambda}(\mathbf{r}_e, \mathbf{r}_h)$$

Developed VR tools

- Viewers for specific chemical systems
 - Molecular dynamics simulation (4D dataset)
 - Exploration of electron-hole interactions (6D)
- Running on various VR devices; interaction and rendering tailored for each device



Supported Hardware



- LRZ CAVE-like system
- HTC Vive
- Samsung GearVR



User Study

- Informal talks with non-experts
- 14-item post-questionnaire for experts
- 15 domain experts
- Questions regarding navigation, interaction, data understanding, ease-of-use, students use
- $4,683 \pm 1,997$, $t=2,65$ (2σ), 7-point Likert scale: slight, but significant, preference for the VR system.

Future work

- Generalization of the demos and integration in the NOMAD infrastructure
- Addition of new functionality and chemical systems
- Increase ease of use: More intuitive interface and more extensive documentation
- Outreach activities

GearVR demo and questions

