



# Materials Design

## 2024 UGM Webinar Series

An Interview with Professor Sir Richard Catlow FRS

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University College London

Cardiff University

Fellow of the Royal Society of Chemistry

October 29, 2024





# Materials Design UGM

# UGM 2024

*The Materials Design annual user event will be online for 2024.*

*Tuesdays and Thursdays  
October 15 – November 7*

*Plenary Speakers:*

***Professor Sir Richard Catlow - University College London, England***

***Professor Georg Kresse, Dr. Martijn Marsman,  
and Dr. Manuel Engel - The University of Vienna, Austria***

***Professor Greg Olson - Massachusetts Institute of Technology, USA***

***Dr. Céline Chizallet - IFP Energies Nouvelles, France***

<https://ugm.materialsdesign.com/>



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# Webinar Speakers

*Katherine Hollingsworth*

*Dr. Erich Wimmer*

# Materials Design UGM Presenter



Professor Sir Richard Catlow FRS

University College London

Cardiff University

Fellow of the Royal Society of Chemistry

# Materials Design UGM Webinar Series

- Share the plenary sessions with your colleagues!

- Registration details

<https://www.ugm.materialsdesign.com>

- We will be recording this session

- Upcoming sessions are posted on the UGM site

- Watch any of our earlier webinars anytime [www.materialsdesign.com/webinars](http://www.materialsdesign.com/webinars)

- Brief survey

- Take a 2 minutes brief survey at the end of the webinar

- Audio issues

- Log out and log back in again

- Check your audio output

- Google Chrome (most recent 2 versions) Mozilla Firefox (most recent 2 versions) Apple Safari (most recent 2 versions) Microsoft Edge (most recent 2 versions)

# Please Ask Questions!

The screenshot shows a Zoom meeting interface. At the top, the name 'Shubham Pandey' is visible next to a microphone icon. The top right corner shows the time '15:23:39' and a chat icon. A green oval with an upward-pointing arrow contains the text 'Type your questions here'. The main content area shows a video feed of Shubham Pandey and a shared browser window. The browser window displays a plot titled 'Estimated Error of the Energy' with the following data series:

Simulation time (MD time steps)	Bayesian error (eV/atom)	RMS error (eV/atom)
0	0.16	0.16
200	0.14	0.14
400	0.12	0.12
600	0.10	0.10
800	0.08	0.08
1000	0.06	0.06
1200	0.04	0.04
1400	0.04	0.04
1600	0.04	0.04
1800	0.04	0.04
2000	0.04	0.04

The plot also shows a red line representing 'Bayesian error' and a blue line representing 'RMS error'. The x-axis is 'Simulation time (MD time steps)' from 0 to 2000. The left y-axis is 'Bayesian error of energy (eV/atom)' from 0.02 to 0.18. The right y-axis is 'RMS error of energy (eV/atom)' from 8 to 8.7. The browser window title is 'JobServer Home Summary Jobs Administration Documentation Mpi/desktop-Stagok --v3.18.24100215 2024-10-17 12:36:54'. The browser address bar shows 'localhost:20202@stagnation:~/JobServer/~/Stagok/~/MLFF\_EnergyErrors'. The bottom of the Zoom interface shows controls for Record, React, Mic, Camera, Share, Leave, and Captions.

# Question and Answer Session



***Dr. Erich Wimmer***

*Materials Design*



***Professor Sir Richard Catlow FRS***

*University College London and Cardiff University*

# Announcements

[ugm.materialsdesign.com](http://ugm.materialsdesign.com)

***MedeA Training***

***Thursday, October 31<sup>st</sup>***



***Dr. Garrett Tow***  
***Materials Design***

***Next Week's Plenary Session***

***Tuesday, November 5<sup>th</sup>***



***Professor Georg Kresse, Dr. Martijn Marsman and Dr. Manuel Engel***  
***University of Vienna and VASP GmbH***

# Question and Answer Session



***Dr. Erich Wimmer***

*Materials Design*



***Professor Sir Richard Catlow FRS***

*University College London and Cardiff University*

# Questions about Materials Design UGM

***Katherine Hollingsworth***

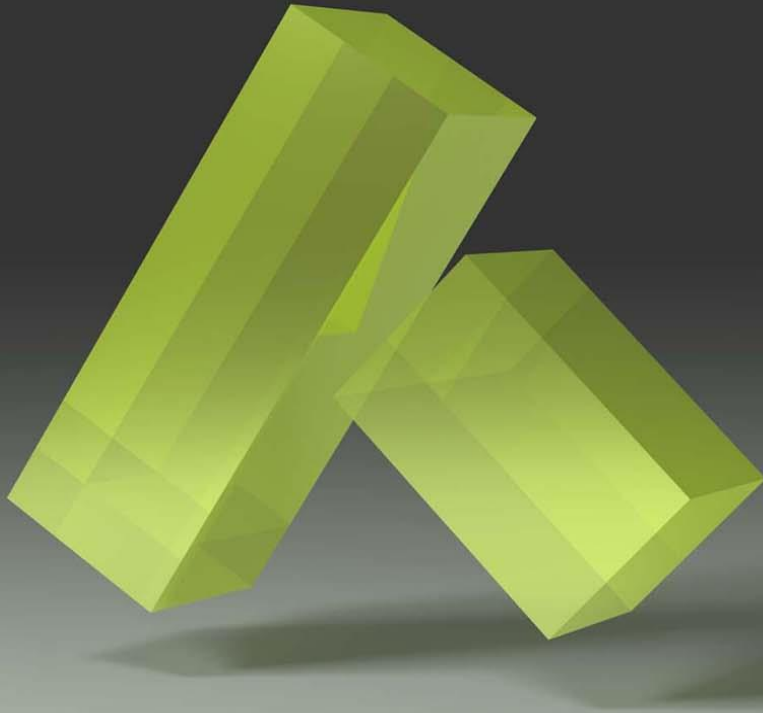
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**materials design**

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# *MedeA*

Innovation by Simulation