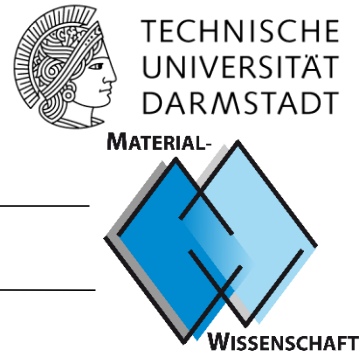


# Materialwissenschaftliches Kolloquium



Montag, 16. März 2020, 15:20 Uhr s.t., L2/01 Raum 77



**Prof. Keith Patrick McKenna**

*Department of Physics*

*University of York*

*keith.mckenna@york.ac.uk*

## *Structure and properties of extended defects through first principles calculations and electron microscopy*

Semiconducting and insulating materials are ubiquitous in nature and find diverse applications in technology. Such materials are normally polycrystalline and contain extended defects such as grain boundaries and dislocations that can affect their properties. While the role of such defects on mechanical properties is relatively well understood their impact on electronic, optical, magnetic or chemical properties is far less clear and challenging to probe experimentally. In this talk, I will present some of our recent work on modelling the structure and properties of extended defects in a range of materials of practical and fundamental interest using first principles methods. These materials include  $\text{TiO}_2$  [1,2],  $\text{MgO}$  [3-5],  $\text{Fe}_3\text{O}_4$  [6,7], formamidinium lead iodide [8] and  $\text{HfO}_2$  [9] and in each case links to complementary experimental transmission electron microscopy investigations will be highlighted.

### References

- [1] E. Maras et al, *Acta Materialia* **163**, 199 (2018)
- [2] J. Quirk, V. Lazarov and K. P. McKenna, *Advanced Theory and Simulations* **2**, 1900157 (2019)
- [3] Z-C. Wang et al, *Nature* **479**, 380-383 (2011)
- [4] Z-C. Wang et al, *Nature Communications* **5**, 3239 (2014)
- [5] J. J. Bean et al, *Scientific Reports* **7**, 45594 (2017)
- [6] K. P. McKenna et al, *Nature Communications* **5**, 5740 (2014)
- [7] N. Fontaina-Troitino et al, *Journal of Materials Chemistry C* **6**, 12800 (2018)
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- [9] S. Petzold et al, *Advanced Electronic Materials* **5**, 1900484 (2019)

Nach Vortrag Diskussion bei Bier und Brezeln. Eine mögliche Nachsitzung wird mündlich angekündigt.