

Masterarbeit: Spintro-Catalysis on RuO₂ (110)

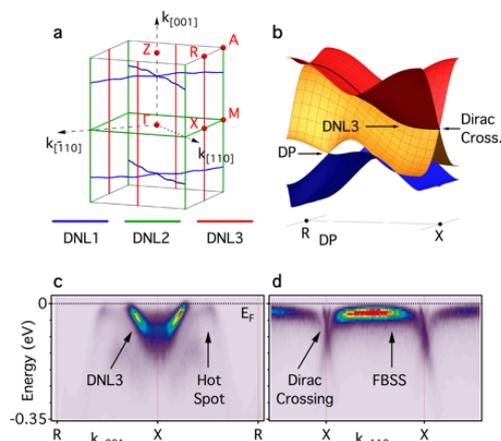


Fig 1: ARPES measurements on RuO₂ show Dirac Nodal Lines (DNL) and Flat band surface state (FBSS).

A new research area at the chair of EP IV at JMU aims at bridging the gap between the fundamental topological- and the applied catalytic properties of topological materials. A prime candidate of our active investigation is the Dirac semimetal RuO₂,¹ found to exhibit a series of unusual physical phenomena such as colinear antiferromagnetism,² the crystal Hall effect^{3,4} and Dirac Nodal lines (DNL) along with a flat band surface state (FBSS) at the (110) surface.¹ The (110) surface of RuO₂, in particular, is known as the *gold standard* catalyst for the oxygen evolution reaction in electrolytic⁵ and photocatalytic water splitting, the bottleneck reaction in the current quest of hydrogen based renewable energy.⁶ Most interestingly, this exceptional catalytic activity is believed to directly relate to the fundamental electronic

and magnetic properties of RuO₂,⁷ which we seek to demonstrate in this project.

To this end, we have fully characterized the surface electronic structure of RuO₂¹ and are – in collaboration with collaborators in Dresden – about to characterize the fundamental magnetic and transport properties. Our successful epitaxial growth program (Philipp Kessler) reliably provides us with large scale atomically ordered and thickness controlled RuO₂ (110) films, perfectly suited for both the fundamental as well as applied questions at hand.

In this master, the student will **build and characterize a basic electrochemical testing setup with collaboration partners in New Zealand**, to systematically and controllably measure the overpotential in the anodic evolution of oxygen as a function of RuO₂ film crystallinity, thickness, stoichiometry, and crystalline orientation that the student will grow by **pulsed laser deposition (PLD)** and characterize by top notch **in- and ex-situ characterization methods (XPS, LEED, RHEED, XRD, STM)**. Most importantly, we will build a novel type of **electrochemical hydrogen cell under externally applied magnetic field**, thereby controlling the antiferromagnetic Neel order in RuO₂, and according to predictions altering the catalytic overpotential.⁷

1. Jovic, V. *et al.* Dirac nodal lines and flat-band surface state in the functional oxide RuO₂. *Phys. Rev. B* **98**, 241101 (2018).
2. Berlijn, T. *et al.* Itinerant Antiferromagnetism in RuO₂. *Phys. Rev. Lett.* **118**, 077201 (2017).
3. Šmejkal, L., González-Hernández, R., Jungwirth, T., Sinova, J. & Gonz, R. Crystal Hall effect in Collinear Antiferromagnets. 1–10 (2019).
4. Feng, Z. *et al.* Observation of the Crystal Hall Effect in a Collinear Antiferromagnet. 1–24 (2020).
5. Lee, Y., Suntivich, J., May, K. J., Perry, E. E. & Shao-Horn, Y. Synthesis and Activities of Rutile IrO₂ and RuO₂ Nanoparticles for Oxygen Evolution in Acid and Alkaline Solutions. *J. Phys. Chem. Lett.* **3**, 399–404 (2012).
6. Over, H. Surface Chemistry of Ruthenium Dioxide in Heterogeneous Catalysis and Electrocatalysis: From Fundamental to Applied Research. *Chem. Rev.* **112**, 3356–3426 (2012).
7. Torun, E., Fang, C. M., de Wijs, G. a. & de Groot, R. a. Role of Magnetism in Catalysis: RuO₂ (110) Surface. *J. Phys. Chem. C* **117**, 6353–6357 (2013).

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