IAP Seminar

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Tuesday, 6th November 2018, 16:00 s.t.
TU Wien, Institut für Angewandte Physik, E134
1040 Wien, Wiedner Hauptstraße 8-10
Yellow Tower „B“, 5th floor, SEM.R. DB gelb 05 B

Water-oxidation on hematite: insights and some remaining challenges

Hematite is considered a promising material for the water-oxidation reaction. This fact is not surprising given that (i) hematite can theoretically absorb up to 40% of solar radiation, (ii) it shows excellent (photo)electrochemical stability in a pH range from 3 to 14, and (iii) iron is the fourth most abundant element in the Earth's crust. However, so far the reported solar-to-hydrogen conversion efficiency is far from the theoretical limit [1]. Major factors hampering the performance of Fe_2O_3 are high recombination rate and poor oxygen evolution kinetics [2].

Here, I will account for some of our latest effort in understanding the water-oxidation reaction on hematite [3-6]. It will range from comments on the modeling methodology to details of how to improve the reaction kinetics with the help of dopants and intrinsic electric fields. More importantly, I will highlight some of the remaining challenges, which calls for the combination of first-principles calculations and surface science experiments.

[1]: D. K. Bora, A. Braun, E. C. Constable, *Energy Environ. Sci.*, 2013, 6, 407-425.
[2]: B. Iandolo, B. Wickman, I. Zorić, A. Hellman, *Journal of Materials Chemistry A* 3, 16896 (2015)
[3]: A. Hellman, B. Iandolo, B. Wickman, H. Grönbeck, J. Baltrusaitis, *Surface Science* 640, 45 (2015)
[4]: B. Iandolo, B. Wickman, E. Svensson, D. Paulsson, A. Hellman, *Nano letters* 16, 2381 (2016)
[5]: R. B. Wang, A. Hellman, *The Journal of Chemical Physics* 148, 094705 (2018)
[6]: R. B. Wang, A. Hellman, *Journal of Physics: Condensed Matter* 30, 275002 (2018)

All interested colleagues are welcome to this seminar lecture (45 min. presentation followed by discussion)

Friedrich Aumayr
(LVA-Leiter)

Gareth Parkinson
(Seminar Chair)