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Regensburg,
18.9.2019

Referee Report on the Habilitation of Dr. Martin Setvin

Dear Members of the Habilitation Committee,

With Dr. Martin Setvin I have a personal acquaintance from several conferences and two visits of our labs, one some years ago the other more recently. It is with great professional interest that I have followed his scientific contributions over the past years, and in preparation of this report I have studied his scientific work in more detail.

Since March 2012 Dr. Martin Setvin has been pursuing his research at the TU Wien (also Vienna University of Technology), where he concentrated on scanning probe microscopy of catalytically relevant oxide surfaces. Catalysis on oxide surfaces is ruled by the presence of defects, excess charge, and by charge transfer between defects, the surface and the reactants. Consequently, Dr. Setvin's research was focused on the interplay of the above-mentioned processes on model oxide systems, foremost the surfaces of rutile and anatase titania. He studied the atomistic aspects of many very fundamental questions in this context. For example, in one of his pioneering works, he could demonstrate that there is a qualitative difference in the localization of excess charges in rutile and anatase titania. In particular, the subtle balance between localization and delocalization for these two very similar systems renders this work a benchmark for current and future theoretical investigations. Other examples of his seminal works include studies of the direct, real-space observation of electron transfer between adsorbates and substrate, the step-by-step atomistic investigation of an on-surface reduction reaction as well as the migration of vacancies and their interaction with charges and step edges.

Dr. Setvin's research shows a very good degree of focus. On the one hand, the research is broad enough to appeal to a wide research community at the interface between physics and chemistry, as is also documented by the many high-impact publications.

On the other hand, it also becomes clear that Dr. Setvin is not just cherry picking from hot topics, but rather following a clearly defined agenda as he addresses overarching research goals in his studies.

Remarkably, instead of merely optimizing a specific catalytic challenge, he contributes to very fundamental questions, as for example, the aforementioned subtle balance between localization and delocalization of charge in the context of polarons. The appreciation from within the community becomes apparent from very high citation counts within a short period of time. This particular work on charge localization in *Physical Review Letters* has been cited more than 180 times in only five years. Similarly, another of Dr. Setvin's work from 2013 has already more than 230 citations.

These two works are the most cited, yet Dr. Setvin's overall citation index is impressive, with a rising trend. Strikingly, in many of the most relevant publications from the past few years, Dr. Martin Setvin is first author, underlining that he has been the main driving force behind this research.

Not only are his research publications highly cited, they are also inspiring due to the fundamental issues that are discussed in a clear manner.

In the context of a habilitation, teaching quality should also play an important role. In this respect, I obviously lack first-hand knowledge of Dr. Setvin's teaching abilities. However, for a similar report, I had access to the students' evaluations of Dr. Setvin's courses held at the TU Wien. He received very good ratings throughout and I should like to emphasize that students' comments like "the best tutor that one could ever wish for" speak for themselves.

In conclusion, I wish to express without any hesitation my absolute strongest recommendation for the habilitation of Dr. Martin Setvin and for appointing him as an associate professor.

In fact, I am looking forward to the exciting scientific works of Dr. Martin Setvin in the future.

Sincerely,

