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המחלקה לפיסיקה כימית וביולוגית

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Report on the habilitation thesis of Dr. Viktor Johanek:

This letter is intended to be a critical, fair, and objective assessment of the habilitation thesis entitled "Reaction at Surfaces: From Macroscopic to Molecular Level". Before I discuss it further, let me introduce myself. I am a Senior Scientist (equivalent to an Assistant Professor in the US academic system) at the Weizmann Institute of Science, Israel since 2017. The academia in Israel does not have the Central European habilitation system, and is fully adapted to the American tenure-track system. Nevertheless, I am generally familiar with how the habilitation system works thanks to a part of my past career being in Switzerland. I understand that this habilitation thesis is comprised of outputs from multiple positions as a postdoctoral researcher and then as a senior research associate over the past 20 years.

The emphasis of the habilitation thesis and the papers attached are on various surface science experiments (adsorption, co-adsorption, model reactions) mostly on model oxide and metal/oxide surfaces. Overall, the quality of the habilitation thesis and the papers is high. The experimental methodology used in these studies is sound. The structure of the thesis is excellent and it is easy to follow. The papers that comprise the thesis are all original studies with decent to high significance in the surface science field. The (auto) plagiarism audit (Turnitin report) did not indicate a scientific error regarding copying.

The following are the highlights of the thesis:

- Size-dependency of fluctuation and bistability on nanoparticles

- Activation of water, activation and conversion of some alcohols and other oxygenates on ceria and metal/ceria surfaces (as matter of fact, Dr. Johanek has a very good contribution to the surface chemistry on ceria)

Other studies in the thesis include:

- Several studies on graphene growth

- Several studies on CO oxidation and NO_x reduction

Dr. Johanek's research involves a masterful use of scientific equipment and vacuum tools. Throughout their career, multiple surface-sensitive spectroscopy and microscopy techniques were employed (such as x-ray photoelectron spectroscopy (XPS), infrared reflection absorption spectroscopy (IRRAS), scanning tunneling microscopy (STM), thermal desorption spectroscopy (TDS), combination of molecular beams and mass spectroscopy (MS) to name a few). I would argue that

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diffraction/scattering experiments in surface science (and in all physical, chemical, and life sciences) are as important as spectroscopy and microscopy experiments, but Dr. Johanek does not mention this in their excellently written introduction. There are also some scientific points that I would like to raise:

- Most of the presented work is either on experiments in UHV or reaction studies with particles. There is, however, an emphasis in the introduction on the ambient pressure techniques, but the only example I can find is some parts of the study in appendix 15. I can see in the outlook section that Dr. Johanek is planning to switch to experiments at ambient pressure in the future, but I cannot consider Dr. Johanek an expert in these novel approaches. Beam-induced effects and cross-contamination are major issues in these novel approaches at ambient pressures. For instance, on page 14 Dr. Johanek speculates that there are restrictions to perform experiments with STM at ambient pressures; however, as explained in ref. 638, this is not the case. In fact, STM is not an invasive technique, which makes it more reliable than electron microscopy. STM is also preferred over atomic force microscopy (AFM) at ambient pressures because AFM resolution decreases with air damping. This argument shows a slight lack of knowledge regarding the pros and cons of all these novel approaches.

- Time-resolved IRRAS is an interesting technique, but I find it misleading calling modulation-demodulation techniques time-resolved. These are not pump-probe measurements on the phase signal. There is no time-resolution on the process, rather the process is modulated in real-time (in terms of chemistry, it translates to most standard reactions being in equilibrium but the modulated reaction being in non-equilibrium conditions).

- From what I understand, there are many papers out there in the literature suggesting the irreversible oxidation of the partially reduced ceria surfaces upon recombinative desorption of hydroxyls as hydrogen, whereas Dr. Johanek suggests reversible oxidation of partially reduced surface upon recombinative desorption of hydroxyls as water vapor. These are conflicting claims. Does Dr. Johanek think all the other papers out there with TDS, XPS, and other techniques are wrong? I am aware that they think that ceria should be strongly reduced (as opposed to partially reduced) to be oxidized in the presence of water vapor.

- Page 42: CO_2 can be produced both by partial oxidation of methanol (desired mechanism) or full oxidation (highly undesired). I am not sure however, how we are supposed to compare it to CO oxidation, which has only one reaction pathway. I find 'CO oxidation' as a model reaction to be a very naïve approach. CO and methanol (or methoxy) are very different molecules, attaching to the surface from carbon in one case and oxygen in the other case. The electronic interaction with the surface is entirely different. I understand that both the $2\pi^*$ orbital of CO and the 2e orbital of methoxy are C–O antibonding in character and adsorption on a metal weakens this bond, but is this enough for a fair comparison of both processes?

To conclude my remarks, Dr. Johanek's contributions to surface science are significant and their studies are of the highest quality. However, I am not sure if this collection of studies will be awarded a

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tenured position in my institute, Weizmann Institute of Science, because of two reasons: 1- there is not enough independent work (i.e., not enough articles where Dr. Johanek is the first or the corresponding author), 2- not enough 'trademark studies' that other scientists in the surface science field will immediately associate it with Dr. Johanek upon first seeing them. It is up to the committee members of the Charles University to decide whether such criteria are important for them. If they are not as important as in my institute, then I recommend the acceptance of the thesis. If the opposite is true, then they should take this into account. There are also some scientific aspects that are listed above that require further elaboration.

Dr. Baran Eren

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