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Evaluation report on the Habilitation thesis

"Electronic relaxation of low-energy metastable states of atomic and molecular systems"

by Dr. Premysl Kolorenc

The habilitation thesis by Dr. Premysl Kolerenc summarizes his research in the field of theoretical chemistry on electronic relaxation processes in atomic and molecular systems. Whenever electronic systems are excited into an intermediate metastable state, they will relax back to the equilibrium ground state via various electronic and nuclear relaxation processes. While processes like radiative decay or internal conversion are quite well studied, Dr. Kolerenc focused on electronic decay processes, which in most cases involve the emission of an electron. In other words, all projects of Dr. Kolerenc deal with electronically unstable systems, which are extremely challenging for electronic structure calculations. The reason for this is the requirement to not only pay attention to the investigated molecule but also to the electronic continuum, into which the electronic state of interest is embedded. The performed high-level and state-of-the-art calculations performed by Dr. Kolerenc address this problem in very elegant ways, and thus allow him to gain valuable insight into the studied molecular and atomic spectra, but moreover into unprecedented electronic decay process like intermolecular Coulomb decay.

I have also gone through the check of originality of the thesis provided by the system Turnitin and it makes undoubtedly clear that the thesis represents an original work of Dr. Kolerenc. The only overlap exists with the published literature that has been written by himself. Hence, the Turnitin report did not indicate scientific misconduct regarding copying in any sense.



The scientific contributions of Dr. Kolerenc are summarized in fifteen publications that appeared in renowned international journals. They are very original and each single one is an important contribution and step forward in the field of electronic resonances. However, the listed fifteen original publications span a timeframe of 11 years from 2009 to 2020 and, on most of them, an established scientist (Averbukh or Cederbaum) is also co-author and often even the responsible last author. In the German academic system, independent research and publications are important ingredients for a successful habilitation, and this requirement would at least be critically discussed in a German habilitation committee given the listed fifteen publications by Dr. Kolorenc.

The thesis itself is excellently written and fulfills in all aspects the highest standards of scientific writing. The scientific training of Dr. Kolorenc is beyond any doubt excellent having worked with the World leading experts in the theoretical investigation of atomic and molecular resonances. I have myself heard scientific talks by Dr. Kolorenc on several occasions and experienced him as a dedicated scientist and talented presenter. Therefore, I am convinced he possesses all credentials to pursue an academic career successfully. In summary, I suggest to accept his habilitation thesis despite my slight criticism concerning his scientific independence, since Dr. Kolorenc's other qualities overweight this clearly.

Sincerely,



Prof. Dr. Andreas Dreuw