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Review

on the habilitation thesis of Ing. Ivan Nemec, Ph.D., entitled
***From Crystallography to Quantum Crystallography of Magnetically Bistable Materials**,*
submitted to Palacký University Olomouc

I received the text of habilitation thesis prepared by Ing. Ivan Nemec, Ph.D., (Palacký University Olomouc; Central European Institute of Technology CEITEC) in the form of a guide through the selected 10 articles co-authored by the candidate, published within the 2020-2023 period in the peer-reviewed journals and disclosing the new scholarly findings, accompanied by the appropriate co-authors' statements. I also received other documents showing the complete list of published works and course of his carrier development including scientific research, teaching, training, and students supervising. As the active researcher in the field of molecular compounds and materials involving the interest in magnetic materials, hereby I provide the review according to the agreement with the authorities of the promoting institution.

The submitted habilitation thesis describes the research of the candidate in the field of magnetic molecular materials based on coordination complexes involving single-ion magnets (SIM) and spin-crossover (SCO) compounds. Those two groups of compounds are currently dynamically exploited in the pursuit of switchable nanoscale object ready to be incorporated into minimized electronic/spintronic nanodevices, exploiting single molecules or their nanoaggregates for ultrahigh density information processing and storage, and quantum computing. SIM and SCO compounds have a potential to provide various controllable spin state as the platform for quantum operation under external conditions. The theory underlying the processes and applications including the conditions to achieve the proper magnetic anisotropy properties (SIMs) or proper crystal filed and cooperativity (SCO) together with the nowadays requirements and milestones were properly described in Ch. 1. The author distinguished the role non-covalent interactions in shaping the properties, which conforms the current trends, in line with the current demands. Then, Ch. 2 and Ch. 3 were dedicated to the detailed description of the results achieved within 10 selected articles.

The candidate uses the range of the dedicated techniques to properly describe his solid state phases and to reach correlation between the crystal structure and magnetic properties: SC XRD, PXRD, dc and ac SQUID magnetometry, the full range of EPR techniques (various bands and HF-EPR), and others, all involving experiments and fitting or simulations. The development of crystallographic description forms the axis of the candidate's research and submitted thesis.

One of the strong points of the performed research is a focus on the role of specific non-covalent interactions in shaping the properties. Hereby, my duty is to distinguish the description of the role of traditional hydrogen bonds, π-π interactions, regium and spodium bonds, halogen bonds and interactions of complexes with anions, as well as non-typical bonds involving directly the metal ion through semi-coordination bonds or metal···π interactions. Moreover, the candidate uses various state-of-the-art computational methods appointed to describe the key phenomena in SIM and SCO species: DFT (deformation and transfer of electronic density, spin density), QT-AIM approach, NCI analysis, DoS diagrams, and separation energy. The key platforms for the magnetic properties, namely the splitting of *d* orbitals in various crystal field and the subsequent ladders of the Kramers doublets (the latter ones crucial for SIM properties) are described by the *ab initio* methods using various orbitals bases. The proper scheme is appointed, involving the stereochemical non-rigidity of the coordination spheres (due to the change of coordination number or the change in coordination polyhedron, both described by SHAPE method) implied either by the impact of supramolecular contacts and by the specific features of judiciously selected ligand.

Another important virtue of the thesis are the attempts to deposit the magnetically active molecules on the surfaces to produce the nanoscale composite. This is an inevitable step nowadays, as such studies allow minimization approach, to assess the real potential of the active molecular modules in abovementioned applications. This includes construction of thin films on the Au(111) surfaces, embedment in polymeric matrices, deposition on graphene, thermal sublimation (*via* engaging the metallocene appends) combined with lithographically controlled wetting or optical microimaging. The selected molecules were made volatile through the attachment of the suitable organometallic module.

Finally, the crystallization rate being more physical than chemical factor is considered as a feature conditioning subtly the SIM and SCO properties, due to its possible influence on crystal lattice defects that might be decisive.

I fully appreciate the construction and the contents of the submitted habilitation thesis as a proper example of the scientific and academic career account and this stage.

To describe the candidate, basing on my knowledge about the articles included in the thesis, the co-authors' statements, and other submitted documents, as well as on the recognition of his activity in the field (conferences presentations, peer-review activity, external scientific stays), below I would like express the virtues of the candidate:

- A growing scientific personality and inner strength to follow on dynamically;
- Attracting young scientists to the science;
- A tendency to equally specialize in various aspects of scientific work: design and synthesis, conducting measurements and computation as well as data analysis and manuscript preparation;
- Acknowledgement by important and influential personalities in the field over Europe and cooperation with the recognized groups.
- A strict and vigilant observer of the nature with a critical view on his own work, able to plan the future work to develop further his skills according to the demands in the field (as was summarized in Ch. 4)

To describe in details of the candidate's involvement into the preparation of the selected 10 publications I would like to list the type of involvement and the positioning of his names among the authors together with the frequency of occurrence: *Corresponding author*: 8 articles (2 times together with other colleagues); *First author*: 4 articles; *Last author*: 1 article; *Project administration*: 7 articles; *Conceptualization*: 9 articles; *Supervision*: 7 articles; *Investigation*: 8 articles; *Formal analysis*: 9 articles; *Writing – original drafts*: 10 articles (complete).

The above information clearly indicates the scientific maturity of the candidate and his readiness to lead his own group within his future research.

Going beyond the scope of this review, I would like to express my appreciation to the total scientific and academic score of the candidate.

As far as the questions to the candidate are concerned (i.e. those which might be addressed during the public defense) I would be glad to receive information, which aspects of his hitherto work would be important if he decided to incorporate lanthanide and actinide ions complexes into his own research program.

To conclude, acting as the appointed reviewer, herein I **definitely support** awarding Ing. Ivan Nemec, Ph.D., the degree of habilitated doctor and promoting him to the associate professorship according to the applicable law in Czech Republic (the Higher Education Act) represented by the regulations at the Faculty of Science of the Palacký University Olomouc (Sections 30, 71 - 75 of Act No. 111/1998 Sb.).

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