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How to Design, Write, and Publish a Scientific Article: A Short Guide Based on the QTNano Group Experience – November 6, 2022

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Abstract

Scientific writing is the technical writing employed by scientists world wide to communicate their research to the scientific community. Thus, it has a special style to communicate the motivation, technical methods, facts, results, insights, and discussion, and hence, it is a challenge for many researchers, in particular, for the beginners in the field, e.g., master and PhD students, as well as for fresh postdocs. In this white paper,* we summarize procedures, strategies, and recommendations to write a scientific manuscript employed by the QTNano (Quantum Theory of Nanomaterials) Group – Juarez L. F. Da Silva,[†] which were collected along several years of experience and more than 200 scientific publications in international journals.[‡] It summarizes only the success procedures, strategies, and recommendations, while the failure cases are not mentioned or discussed in this document, however, those cases were crucial to improve our procedures and strategies at the QTNano

group. Furthermore, the present document benefits also from several short or long papers on scientific writing, which were studied along the years. Therefore, following this document may help you to write a solid and well organized manuscript within the QTNano group, which can improve your chance to obtain a good publication at the end. For last, it is a work in progress, which has been improved semester by semester. The present version was compiled on November 6, 2022.

Abbreviations

QTNano, VASP, FHI-aims, LAMMPS, Gromacs, ORCID, Gnuplot, Grace, QtGrace, VESTA, etc.

Keywords

QTNano Group, Scientific Writing, Literature Review, QTNano Project Concept, Citations, Files organization, References, Data Management, Academic Integrity, Latex, Supporting Information, Reply Letter, Scientific Journals, Reviewers

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* As summarized at [Wikipedia](#), a white paper is an authoritative report or guide that informs readers concisely about a complex issue and presents the issuing body's philosophy on the matter. It is meant to help readers understand an issue, solve a problem, or make a decision. † Originally, the Juarez L. F. Da Silva's group started at the São Carlos Institute of Physics, University of São Paulo, on August 2009, supported by a [Young Research FAPESP grant](#). It was transferred to the São Carlos Institute of Chemistry, University of São Paulo (at the same Campus) on May 18, 2012, where Juarez L. F. Da Silva started his first faculty position. The name "QTNano group – Juarez L. F. Da Silva" was adopted from January 2014.

‡ For additional information on the behalf of Juarez L. F. Da Silva, see links <https://linktr.ee/juarezlfdasilva> and <https://linktr.ee/QTNano>.

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1 QTNano Members: Why Do You Need to Read this Document?

We will start this white paper by searching the combination of two words, **Scientific Writing**, at the world wide web (www) library using the **Google search engine**, which can yield several initial links with useful information. From that, we can notice two important facts: (i) There are too many good www links and it is impossible to check (read) all of them in hours, days, or even years. (ii) It is very hard to find a link, which can provide all important details and procedures to write a paper within a particular field, e.g., chemistry, physics, computational material science, computer science, biology, etc.

Everyone can use a general recipe to write and publish a scientific paper, however, the authors will have to face few challenges to reach their goals. For example, every research field has their own style for data organization, discussions,

technical terms, figures, tables, and so on. Furthermore, maybe the most important one, every scientific group has their own style for data organization, manuscript size preference (e.g., letters, regular papers, reviews, etc) time-frame,^{*} software,[†] rules,[‡] and etc, to write and publish their scientific work.

At the same time, it is a challenge for every fresh graduate students and postdocs to start to write his/her first manuscript within a particular research group without a proper guidance on the structure, titles selection, procedures, data organization, etc. Thus, to reduce the barrier for the QTNano group members, we started to write this document[§] to help the QTNano members to achieve their goals, minimize stress, and to improve their education on scientific writing. Furthermore, the present document can be used by different research groups as is it or adjust our procedures for their local group conditions.

2 Scientific Writing: Why Is It So Important?

To continue our discussion, we would like to highlight few outstanding remarks by Prof. Dr. Rick Lombardo, from the University of Nebraska-Lincoln, which are discussed below.

1. *Scientific writing is not just writing about science; it is the technical writing that scientists do to communicate their research to others. Scientific writing is predicated on the rigors of scientific inquiry, so it must reflect the same precision as that demanded in the research process. Scientific communication demands precision (the precise use of words and phrases), clarity, and economy.* At the QTNano group, we have been known to be very accurate in our procedures, calculations, and interpretation of results obtained from *ab initio* or force-field simulations. Thus, our papers should reflect this culture, which implies well

* Write the manuscript only at the end of the project. [†] In general, experimental groups like Microsoft Word, while several theoretical groups have a preference for Latex. It is our case, i.e., we love Latex. [‡] The first author or correspondent author will write the manuscript alone without the feedback from the remaining co-authors. We do not apply this rule within our group, where all authors should contribute based on their position within the author list. [§] We update this document very often, and hence, its version contains the date at the end of the title.

designed Figures to capture the most important findings, well organized Tables, deep and critical discussion of the most important results, and so on.

2. *Many journals have international audiences, so precise communication helps prevent misunderstandings and mistranslations in other contexts. Communicating facts, figures, and methods used in research – as well as the description of the results – has to be precise and exact.* This remark is crucial today and beyond, in particular, because machine learning techniques will read our papers in future and extract additional knowledge from that. Thus, we should be precise on the language and ideas, which is crucial to deliver the expected goal.
3. *The organization of a paper is logical, with rules for what goes into each section. Read papers from your particular discipline to understand the relevant rules. Briefly, your order of presentation should make the most sense to your reader. This is what is commonly referred to as readability.* All new members, should read at least 10 papers from our group before start to write his/her own scientific manuscript, in particular, study the organization of each paper. If possible, organize a meeting to discuss with the first author within the QTNano group all decisions that leads to that particular structure organization.
4. *This is the point where scientific writing most noticeably resembles other types of writing. Logic and organization isn't automatic. It doesn't come naturally from your head to the paper. You need to step back and impose logic on your writing; you then need to crystallize it by always asking yourself this question: "Will this make sense to the reader?" It doesn't matter if it makes sense to you. It must make sense to the reader.* Here, we get to the point in which most of us have great difficulties, and it is the explanation for the delays of several manuscripts. The manuscript must be clear for the readers, who matters at the end.
5. *Every paragraph should have one topic sentence, not two or three. All sentences in a paragraph should support or elaborate upon what your topic sentence says you plan*

to discuss. You should be able to provide a rationale for why each sentence is placed where it is in each paragraph. All of your paragraphs should be logically organized around your section headings or sub-headings. You should have a rationale for where each paragraph is placed. You must maintain a natural logic that is accessible to the reader. Thus, before start to write the manuscript organize a list of the most important results/findings that should be discussed in each section, and then, build up the structure of the section, i.e., from line zero up to the end.

6. *If you can't clearly, concisely, and logically communicate how you collected and analyzed your data, it does not matter how groundbreaking your research is. Readers won't understand it and will justifiably question your results. However, if you can clearly explain your work, it will be understood by more people.* Nowadays, this remarks summarize every thing, i.e., we will not have success in science without good scientific writing. In 2021, Prof. Dr. Prashant Kamat confirmed the same message using different words at the CINE Webinar (online event), Center for Innovation on New Energies.

Thus, every researcher should work hard to improve their scientific writing, which includes a wide range of skills, e.g., write using a foreigner language, logical organization of the most important ideas, well designed figures, table organization, deep understanding of physical-chemistry concepts, results discussion, etc. From my personal opinion, a good writer is the one that never give up to study and improve their skills, which should evolve along our academic career.

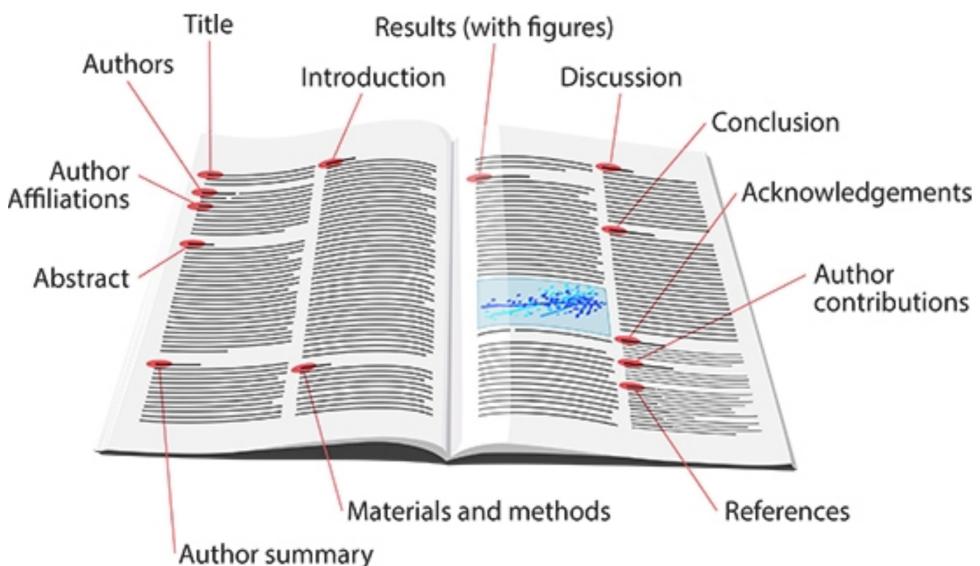
3 Recommended Online Courses

As mentioned above, there are several free online courses to improve your scientific writing,* e.g., see the link at www.clippings.me, where you can find at least five good recommendations.[†]

* This section was based on the suggestions provided by Vivianne Karina Ocampo Restrepo, who concluded her PhD in the QTNano group on March 2022. [†] In case that you have a suggestion for this list, please, get in contact by the following email: juarez_dasilva@iqsc.usp.br.

1. **Stanford University - School of Medicine.** As written in their website, This course teaches scientists to become more effective writers, using practical examples and exercises. Topics include: principles of good writing, tricks for writing faster and with less anxiety, the format of a scientific manuscript, and issues in publication and peer review. Students from non-science disciplines can benefit from the training provided in the first four weeks (on general principles of effective writing).
2. **Nature Master Classes.** 11 hours course with focus on natural science.
3. **Coursera.** 14 hours course.
4. **Duke University.**
5. **Keneckert.** As written in their website, There are many books to help students write in English, but few deal with academic writing at the graduate or high-undergraduate level, and still fewer which address the particular needs of nonnative learners of English. This book explains to the graduate student or senior how to better plan, research, write, and edit an argument seminar paper, thesis/dissertation, or postgraduate scholarly publication in MLA, APA, or IEEE format. While it is tailored to English language learners and especially Koreans, the information here is meant to be helpful for any writer.

Although those courses provide great training and tips to improve your skills on scientific writing in nature science, it is important to keep in mind that scientific writing skills is obtained with hands-on, i.e., you must write several scientific manuscript along with your supervisors and collaborators, who will provide suggestions, acid comments, perform corrections, and revise the manuscript at the end. As mentioned above, scientific writing is a style of writing to communicate scientific work, however, researchers are human kind and develop their own styles, which depends also on the field, e.g., biology, physics, chemistry, etc. Thus, it is very important to keep in mind that several tips and recommendations provided by those courses might apply only in particular fields.



<https://mindthegraph.com/blog/read-scientific-papers/>

Figure 1 Example of the organization used for a regular paper.

4 Paper Basic Structure

A paper can be organized in several different formats, which should take into account the scientific contribution and technical journal requirements. For example, a paper can be classified in review, regular article, letter, perspective, comment, erratum, etc, however, by number, the regular article format is the most employed by the scientific community. It has several sections as shown in Figure 1. Below, we will provide a compact discussion for each part of a regular paper.

4.1 Title

The selection of a good title for a scientific paper is a challenge even for experienced writers, which a deep understanding and broad consequences of the scientific findings. It is important to realize that the title is the gateway to your scientific paper, and it is the first piece of information that will be read by editors, reviewers, and potential readers, which includes human and non-human readers such as PubMed, Google Scholar, Web of science, Scifinder, etc.

At this section, our discussion will be based on the editorial paper written by Prof. Prashant V. Kamat (Editors-in-chief of ACS Energy Letters),¹ who recommend a list of five key attributes of an effective title. For example, the title should be accurate (correct in all details), concise (brief), clear (able to be understood by any potential reader), declarative (states a fact), engaged, and

focused for the editors, reviewers, and potential readers.

As in the study of clusters in quantum-chemistry, where every atom and electron counts, every word counts for a good title. Therefore, it is crucial to capture the main message within the title. Below, we list the five attributes recommend by Prof. Prashant V. Kamat, however, we will consider additional attributes, e.g., What to avoid in the title?

1. **Journal Scope** – the title should match with the journal focus, i.e., broader or specialized journal.
2. **Simplicity** – our goal in science is the translation of complex behavior into simple models, which can be explained for any potential readers. Thus, the title must capture this simplicity, which implies to keep the title as concise as possible. In particular, it is hard to find long titles in broader journals, while longer titles are more common on specialized journals.
3. **Inquisitiveness/Curiosity** – like in Hollywood movies, the title should raise curiosity on the potential readers, and hence, impact statements combined with straightforward messages can be used as a recipe to design good titles.
4. **Conjunctions** – the use and control of the language is essential, which includes the correct use of conjunctions such as *and*,

or, with, instead, for, but, etc, however, it is important avoid its excessive use.

5. **Breaking the Title/Two Parts** – for that cases in which the use of conjunctions is not effective or does not work so well, then, the breaking of the title into two parts can be used as a solution. As expected, we should use it only once.
6. **What to Avoid?** – avoid words such as *Investigation, Study, Demonstration, Novel, Facile, Superior, Highly Efficient, High Efficient*.
7. **How Many Words?** – many ACS journals recommend titles with less than 15 – 20 words. Thus, it can be used as a metric to avoid very long titles.

4.2 Choosing your Scientific Name

We added this topic within the discussion to raise awareness among early careers researchers on the importance of the problem of name ambiguity in the scientific community. For example, problems with names can affect number of citations, *h*-index, and so on, which are descriptors employed to evaluate your projects, scientific career, and so on. Therefore, the consequences are far from the imagination for early career researchers, when the goal is good science.

One of the most common problems are names with prefixes, e.g., **de**, **da**, van, vander, etc, because there is no standard among the journals, editors, authors, etc, to deal with that problem. For example, several languages adopt very long names with one or more than one prefix, which turns the situation complicated to use at scientific publications.

Before the publication of my first paper in Germany, at the Fritz–Haber Institute of the Max–Planck Society, my PhD supervisor (Prof. Dr. Mathias Scheffler) told me – think about your scientific name because you have a long name (Juarez Lopes Ferreira da Silva). Thus, after several searches at the Web of Science on 1999, it was possible to arrive on the following conclusions:

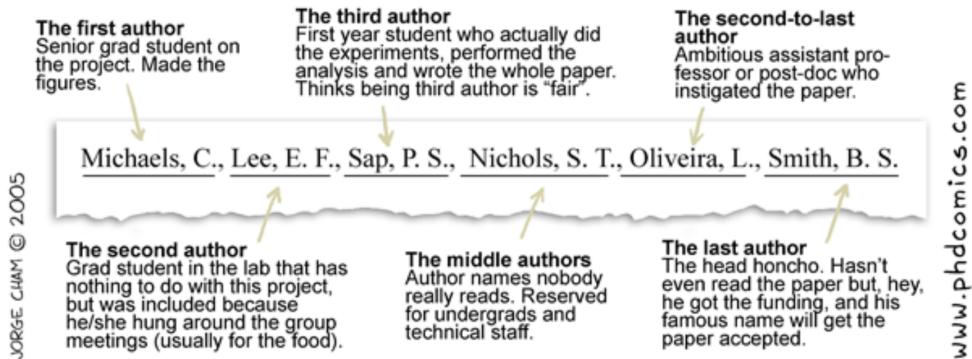
1. Should not use **J. Silva** because there are too many names like that in the scientific literature. Thus, it was not a good idea to reduce the number of words in my name.

2. It was recommended in few places to use the first name as part of the scientific name to avoid similar names. Thus, I decided that **Juarez** should be part of my scientific name.
3. Then, along the searches, it was possible to realize a problem with the prefix **da**, which is part of my name. Checking the name of several authors with similar problem, e.g., **da Silva**, was possible to notice that in several citations or list of authors the prefix **da** was employed or not employed in different cases. Furthermore, that time, I did not find a standard procedure to deal with that.
4. Thus, at the end of the task, 3 possible suggestions were on the table, namely, Juarez L. Ferreira or Juarez L. F. da Silva or Juarez L. F. Da Silva. Thus, at the end, we selected Juarez L. F. Da Silva because it sounds better and maintains the name structure, however, the prefix was changed and employed like that for all papers, abstracts, posters, web documents, etc. It is an unique name within the scientific community. For citations, my name should be cited as J. L. F. Da Silva or Da Silva, J. L. F..

The recommendations above can minimize several problems, however, it cannot solve all problems for researchers from China, Korea, Japan, etc, where several authors have very similar names or even identical scientific names. Thus, it is one of the reasons to use the Open Researcher and Contributor ID ([ORCID](#)). ORCID as defined in [Wikipedia](#), *is a nonproprietary alphanumeric code to uniquely identify authors and contributors of scholarly communication as well as ORCID's website and services to look up authors and their bibliographic output (and other user-supplied pieces of information)*. It maintained by a non-profit organization and further details can be obtained at the ORCID website, [orcid.org](#).

ORCID has been widely employed by the scientific community to minimize those problems. Therefore, we recommend its creation for all QTNNano members and its connection with every paper submission.

THE AUTHOR LIST: GIVING CREDIT WHERE CREDIT IS DUE



There are comics like that because those situations also happen in real life, and they might look funny when does not happen with us, however, it is our duty to avoid that those behaviors happen in our community, Prof. Dr. Juarez L. F. Da Silva.

<https://www.jakobrdl.dk/blog/2016/08/who-should-be-the-first-author-of-a-scientific-paper>

Figure 2 The author list: a bit of comics, which indicate the challenges to define the author list.

4.3 Authors List

The definition of the author list of a paper is simple once it is done with transparency, integrity, and well defined rules. For example, Figure 2 shows an example of rules, which should not be employed by a scientific group. Therefore, before define the procedures employed by our group, it is important to summarize the most important roles played by the contributors of scholar paper based on the [CRediT \(Contributor Roles Taxonomy\)](#), which includes 14 roles, namely, (i) Conceptualization – Ideas, (ii) Methodology, (iii) Software, (iv) Validation, (v) Formal analysis, (vi) Investigation, (vii) Resources, (viii) Data curation, (ix) Writing – Original Draft, (x) Writing – Review & Editing, (xi) Visualization, (xii) Supervision, (xiii) Project administration, (xiv) Funding acquisition. Thus, several of the authors can play several roles, while a particular author might provide a minor contribution on only one role. Therefore, it is important to report the author contributor statement within every manuscript.

Below, we provide the criteria employed at the QTNano group, which can inspire different groups.

1. In our group, first author is the one that perform most of the job, which includes the following tasks: perform the calculations, data analysis, visualization,

and writing the version zero of the manuscript. That is, it is the author with the larger number of roles within the contributor roles of taxonomy.

2. A group member that writes the manuscript has the priority to be the first author compared with someone that only perform the calculations but cannot write it. Writing the first draft includes several roles, e.g., data organization, data analysis, visualization, etc. Exceptions for that should be discussed carefully before start to write the manuscript.
3. Second, third, and etc, authors are group members or outsiders that provide a contribution to the work within the contributor roles taxonomy, which helps to speed up the work, or an interpretation to improve the discussion of the results.
4. A high quality contribution of 2 hours is enough to justify a contribution as co-author in the manuscript. For example, suppose that a group member is able to explain the results and provide a strong physical and chemical understanding of the problem, which opens the possibility to submit the manuscript for a high quality magazine, and it can be done in two hours, however, every author should contributes

to improve, revise, check the results, discussions, and so on.

5. Once an author is part of the manuscript authors list, then, he/she should be available to revise the manuscript, follow up all changes, improve scientific writing, and help to check the data, which is crucial for every scientific work. In case that an author provides a solid contribution, however, he/she stops to revise the manuscript or do not answer requests to revise, data analysis, data check, and so on, then, he/she should be removed from the authors list. It is a controversy decision, however, we have learned along the years that it is the best procedure to minimize problems.

4.4 Corresponding Author

A common question among fresh graduate and postdocs is related with the procedures to select the corresponding author of a particular paper. According to the Elsevier Authors Service, *the corresponding author is the one individual who takes primary responsibility for communication with the journal during the manuscript submission, peer review, and publication process. Normally, he or she also ensures that all the journal's administrative requirements, such as providing details of authorship, ethics committee approval, clinical trial registration documentation, and gathering conflict of interest forms and statements, are properly completed, although these duties may be delegated to one or more co-authors. Generally, corresponding authors are senior researchers or group leaders with some – or a lot of experience – in the submission and publishing process of scientific research. They are someone who has not only contributed to the paper significantly but also has the ability to ensure that it goes through the publication process smoothly and successfully.*

Therefore, the corresponding author is responsible for several roles along the development of the study and play a critical role at the publication of a manuscript. It is not the rule, but the authors of a particular paper can indicate more than one corresponding author for the situations in which several groups provide equal contribution to the publication. Thus, the electronic mail (E-mail) of the correspondent authors will appear at the paper.

4.5 Abstract

The abstract is one of the most important parts of a paper as it can summarizes several pages of hard scientific work, and hence, the abstract acts as an advertisement for the entire paper. However, many authors do not realize the importance of the abstract, i.e., Why is the abstract so important? The answer for this question is based on our strategies to perform scientific work. For example, along a literature review process at a particular field, we select a large number of scientific papers based on their titles as it is impossible to read all papers. At the sequence, we read the abstract, which should be impressive to keep the attention of potential readers. Thus, the abstract is the first piece of information that any editors, reviewers, and potentials readers will read on your paper and not the last one. Therefore, we should pay attention to write a good abstract. A standard abstract can be composed by following four parts:

1. Problem, importance, and hypothesis – the abstract starts by the presentation of the problem, motivation behind the proposal, hypothesis, and/or a specific question.
2. Methods – it is the easiest part of the abstract, in particular, in the field of computational physics, chemistry, and material science as few technical words can provide and summarize all methods, or at least, the most important ones.
3. Key findings – every scientific work perform several analysis and several findings are identified, which are not equally important. Thus, it is critical to identify the most important highlights obtained in the work, which should be concise and accurate for editors, reviewers, and potential readers. The length of this part depends on the scientific journal, which can limit the number of characters or words.
4. Conclusions or broader implications – most of the abstracts fails at this important as several authors only focus on the highlights, and hence, the consequences of the present work to the field is not provided. In this part, we recommend to avoid words such as, **We believe**

Abstract Title: Mechanistic Exploitation of a Self-Repairing, Blocked Proton Transfer Pathway in an O₂-Tolerant [NiFe]-Hydrogenase

Catalytic long-range proton transfer in [NiFe]-hydrogenases has long been associated with a highly conserved glutamate (E) situated within 4 Å of the active site. We hypothesize that substituting for glutamine (Q) in the O₂-tolerant [NiFe]-hydrogenase-1 from *Escherichia coli* produces a variant (E28Q) with unique properties. These properties have been investigated using protein film electrochemistry, protein film infrared electrochemistry, and X-ray crystallography. At pH 7 and moderate potential, E28Q displays approximately 1% of the activity of the native enzyme, high enough to allow detailed infrared measurements under steady-state conditions. Atomic-level crystal structures reveal partial displacement of the amide side chain by a hydroxide ion, the occupancy of which increases with pH or under oxidizing conditions supporting formation of the superoxidized state of the unusual proximal [4Fe–3S] cluster located nearby. Under these special conditions, the essential exit pathway for at least one of the H⁺ ions produced by H₂ oxidation, and assumed to be blocked in the E28Q variant, is partially repaired. During steady-state H₂ oxidation at neutral pH (i.e., when the barrier to H⁺ exit via Q28 is almost totally closed), the catalytic cycle is dominated by the reduced states “Nia-R” and “Nia-C”, even under highly oxidizing conditions. Hence, E28 is not involved in the initial activation/deprotonation of H₂, but facilitates H⁺ exit later in the catalytic cycle to regenerate the initial oxidized active state, assumed to be Nia-SI. Accordingly, the oxidized inactive resting state, “Ni-B”, is not produced by E28Q in the presence of H₂ at high potential because Nia-SI (the precursor for Ni-B) cannot accumulate. The results have important implications for understanding the catalytic mechanism of [NiFe]-hydrogenases and the control of long-range proton-coupled electron transfer in hydrogenases and other enzymes.

KEY

Abstract contains sufficient background to understand the problem under investigation

Abstract must contain a hypothesis, objective or statement about the problem under investigation

Abstract must contain a brief statement of the experimental methods/methodology used

Essential results must be present in summary form (even if preliminary)

Abstract must contain a conclusion that explains how the work contributes to the hypothesis, objective or statement of problem

Figure 3 Schematic representation for an abstract use in the field of chemistry obtained from www.abrcms.org, which includes all elements discussed below.

4.6 Graphical or Visual Abstract

Everyone has listen the phrase, **A Picture is Worth a Thousand Words**. Nowadays, more than never, this phrase has gained great importance within the scientific community, in particular, for knowledge dissemination of scientific articles within the digital medias, where well designed graphical abstracts can play a crucial role for science dissemination though tweets, Facebook, Linkedin, Journal table of contents, etc.

A graphical or visual abstract of a scientific paper is one single image designed to provide the readers an immediate and deep understanding of the take-home message (key findings and conclusions). Thus, along side the manuscript title, it has the aim to encourage the readers to browse the paper, and hence, it helps also the readers to identify the most relevant topics within their literature search.

Thus, for that, a graphical abstract must be well designed with the take-home message, which should be discussed with all authors along the development of the scientific manuscript. In fact, it should be done at the end, i.e., before

submission. Every scientific journal has their own requirements for the graphical abstract size, which appears along side the abstract in most cases.

4.7 Introduction

The introduction is the entrance gate to your paper, and hence, it should contains all elements to provide a solid and positive impression on any reader (editor, referee, expert in the field, etc). A good introduction has the following elements:

1. **Objectives of the work** – start the introduction with an open paragraph, where we should set up the field, topic.
2. **Justification** – the second or combined with the first paragraph should provide a clear justification for the importance of the work.
3. **Background** – one, two, or several paragraphs that describe the state of the art, and points out a very hot problem that needs to be solved. Then, we should propose our approach to solve

this problem, and provide few results (highlights) that indicates that we were able to solve it. The state-of-the-art is not like, XXX founds this, and YYY found that, and ZZZ found that, which turns the paper horrible to read.

4. **Guidance to the reader** – we should provide a clear direction for our goals within the manuscript, as well as the strategy to address the problem, etc. It is important to be clear and straightforward to the reader.
5. **Summary/Conclusions** – it should contains the most important highlights (key points), which will be reported and discussed along the paper.

4.8 Methodology

The methodology should contains a deep description, discussion, and justification of all the theoretical approach and computational details employed for the study, however, its length size should be appropriate for the manuscript. The methodology should provide all technical details required to reproduce all results within the manuscript by a researcher in the field. Thus, keep in mind that several computational details can be reported within the electronic supporting information file. Furthermore, computational convergence tests can/should be provided within the electronic supporting information file to help the manuscript evaluation and interested readers.

We recommend to give a look in the papers published by the QTNano Group – Juarez L. F. Da Silva to obtain a general perspective on the methodology section, however, the same rules/recommendations can be used by an experimental group. Normally, the methodology section can be composed by few subsections to improve the manuscript organization, which will help potential readers at the end. For example, in computational physics, chemistry, and material science, common subsections are:

1. Total Energy Calculations; Density Functional Theory; Force Field Molecular Dynamics.
2. Atomic Crystal Structures; Clusters Trial Configurations; Adsorption Configurations.

3. Clustering Algorithms for Structure Analyses.
4. Analyses, etc.

4.9 Results and Discussion

The results section is not a description of the results shown in the Figures and Tables. As the title says, **Results and Discussion**, provide a deep understanding and discussion of the data, and comparison with previous results, critical analyses and understanding, etc. A manuscript that only describe the data in the Figures and Tables can takes long time to get submitted within the QTNano Group. Furthermore, it will have a great chance to be rejected by the Editors/Referees.

From our experience, there are several strategies o write the **Results and Discussion** section. Below, we summarize the most common strategies employed by the QTNano Group:

1. Provide the titles for all subsections within this section.
2. Design well organized Figures and Tables that summarizes the most important results, which should fit within all the subsections.
3. Write down within the each subsection the main topics for the discussion (one sentence), and if possible, organize the ideas within well defined paragraphs.
4. Then, write a fast first version for each subsection, where the the most important ideas are written faster.
5. It is like a house, in which the ground is build first (Figures and Tables), and then, we add the pillars (ideas - short sentences), and then, we polish it as much as possible to provide a very good impression for every reader.

4.10 Insights

The Section “Results and Discussion” within a regular paper has a fragmented structure, in which all results are separated into groups and discussed separated or interconnected with solid discussions along the development of the manuscript. However, as consequence, it is a challenge to interconnect all results,

findings, interpretations, and hypothesis in every subsection. Thus, at the QTNNano group, we like to write a solid section before the conclusion section called “Insights”, which has the goal to interconnect all results and findings with experimental observations. Using this approach, the conclusions section should be short and objective, i.e., it should summarize only the keystone results.

4.11 Conclusions

The conclusion should summarize the most important findings and insights obtained by the scientific investigation. Furthermore, it should provide a perspective on the importance of those findings and their consequence to the field, which can help the scientific community. Furthermore, it should be compact, i.e., a maximum of two paragraphs would fit good for most of the papers.

4.12 Acknowledgments

Acknowledgments should be always present in papers, which is usually located after the conclusions section. Commonly, we should acknowledge all economic support provided by the Research Foundations for grants, fellowships, computational resources, etc. Below, we provide the most common statements employed by our group:

1. **FAPESP/Shell:** The authors gratefully acknowledge support from FAPESP (São Paulo Research Foundation, Grant Numbers 2017/11631-2 and 2018/21401-7), Shell and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&D levy regulation.
2. **CAPES:** This study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES) - Finance Code 001 (fellowships for XXX).
3. **CNPq:** This study was financed in part by the National Counsel of Technological and Scientific Development (fellowships for XXX).
4. **LNCC - Santos Dumont:** The authors acknowledge also the National Laboratory

for Scientific Computing (LNCC/MCTI, Brazil) for providing HPC resources of the SDumont supercomputer, which have contributed to the research results reported within this paper. URL: <http://sdumont.lncc.br>.

5. **HPC USP:** QTNNano group acknowledges the Advanced Scientific Computational Laboratory (University of São Paulo) and the infrastructure provided to our computer cluster by the São Carlos Center of Informatics, University of São Paulo.

4.13 Credit Author Statement

As defined by the Elsevier, *CRediT (Contributor Roles Taxonomy) was introduced with the intention of recognizing individual author contributions, reducing authorship disputes and facilitating collaboration. The idea came about following a 2012 collaborative workshop led by Harvard University and the Wellcome Trust, with input from researchers, the International Committee of Medical Journal Editors (ICMJE) and publishers, including Elsevier, represented by Cell Press. CRediT offers authors the opportunity to share an accurate and detailed description of their diverse contributions to the published work. The corresponding author is responsible for ensuring that the descriptions are accurate and agreed by all authors.* For the definition of each role within the contribution roles taxonomy, we recommend to read the original information within the above link.

4.14 References

From our perspective, most of the authors do not put too much attention to the citation process along the production of a paper, which affects everything within a paper. The citations are located at the end of the manuscript, Figure 4, and hence, most of the authors think that it should be done at the end. Last task before complete the manuscript, however, this decision is a big mistake with far consequences, i.e., several mistakes will occur in the references. Normally, along a scientific study, we read and revise several previous studies, and hence, we should keep track of those papers (e.g., list of important papers), which should be cited as required along the process to write the manuscript because it is not possible to remember all those details to include at the end.

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Figure 4 Example of references organization and style employed by the Journal of Applied Energy Materials.

Citing the original sources (papers, books, page at the world wide web, etc) employed in your research have several purposes, namely: (i) It provides proper credit to the original authors of the words, ideas, strategies, methods, etc, that were incorporated into your paper, book, etc. (ii) Furthermore, the readers will have the correct information to cross-check the information directly within the source, which is critical for science reproduction, etc. (iii) Thus, the citation process should be accurate and without errors in the authors names, titles, journal name, page number, year, etc, as those information are employed to count the number of citations for authors, i.e., it has far consequences. (iv) Furthermore, it is crucial to avoid and reduce plagiarism within the scientific community. The present discussion benefited from the ideas discussed within in the [link](#) at the [University of Nebraska Kearney](#).

Along the years, we have identified a large number of problems with citations within a scientific manuscript, which are summarized below:

1. **Over Citations** – It is very common to find a relatively short regular paper with 100 citations, however, a close look identify that 90 % of the citations are located at the introduction and methodology, however, the discussion of the results, the number of citations is only a fraction of the citations. Thus, it is a possible indication that the

authors did not compare their results with previous results from the literature, or compared only slightly. Thus, we considered over citations a problem and it is not recommend at the QTNNano group. At the introduction or methodology, for each statement that requires citation, cite a maximum of two references, but not 5 or even 10 references. We should cite the most important two references, i.e., the first ones that discussed those ideas and provided a real contribution to the field.

2. **Self Citation Problems** – In many cases, a particular paper is based on previous findings or results from an old paper from the QTNNano group, and hence, it deserves to be cited, however, we should not over cite QTNNano papers using a large number of references unless is a review, etc. We should provide always the correct acknowledgment without over citation, which applies for every one within the scientific community.
3. **Bad Citations** – Cite a theoretical paper that contains the experimental data instead of the original experimental paper. This procedure is not accepted and it should not be done at our group.
4. **Track the Correct References** – There are many papers in the literature, which increases almost exponentially along the last decades. Thus, it is a challenge to keep track of every new paper that appears in the literature, and hence, it is crucial to employ automated tools such as Google Scholar or alternative tools to support the organization of your scientific library.

5 How Do You Begin a Paper?

A good scientific paper do not sell numbers or a collection of data (technical report) but a good idea/model/hypotheses, which should be supported by large set of data obtained by well defined procedures. Below, we will discuss two crucial points: (i) paper misconception and the (ii) QTNNano project concept.

5.1 Paper Misconceptions

Most of the fresh graduate students and postdocs think that a scientific paper starts to be written

once all data has been obtained, however, from my personal opinion, it is a wrong concept as data by itself does not contain the questions, hypothesis, etc. A solid paper starts to be written with a solid question/hypothesis, i.e., far before the computational simulations or experimental data acquisition have been done. My PhD project at the Fritz–Haber Institute of the Max–Planck Society (October 1998 up to 04 October 2002) started with the following question: Can you explain the top site preference of Xe adatoms on transition-metal surfaces? A good question/hypothesis can be broken down into several small questions/hypothesis, which can be organized into a solid well defined project. According to the [Cambridge Dictionary](#), a project is *a piece of planned work or an activity that is finished over a period of time and intended to achieve a particular purpose*.

Thus, a scientific project can be composed by a few tasks managed by a single person (graduate student) or thousand tasks, which would require a management organization with multilayer structure composed by principal investigators, co-principal investigators, associated researchers, postdocs, graduate students, and so on. Thus, such large projects can yield a large number of publications, which can be done in parallel by several members of the team. All project tasks can be done sequentially or in parallel mode, however, a project is not only a list of tasks to be done. It must contain the motivation, justification, questions, goals, etc, i.e., the structure of a paper can be designed from beginner, which helps to minimize problems, etc.

5.2 QTNano Project Concept

At most academic or non-academic scientific groups, the group leader provides a well defined question/hypothesis for a new member, which make their life easier at the starting point, however, it induces a lack of understanding and procedures to define a solid paper (project). Except particular institutions, our educational institutions do not provide training on the designing and management of scientific projects for fresh graduate students or even for postdocs. Thus, we must discover the routes by ourselves doing mistakes, studying, experience exchanged, etc.

At the QTNano group, we define the main goals and main ideas/hypotheses before start

the experimental work (calculations), and hence, it provides great help to write the manuscript as the main ideas were previously discussed few times. However, it requires a deep understanding of the scientific field, which requires a solid revision from the literature for fresh graduate and postdocs members. Beyond of that, we should have as many meetings as possible with all co-authors to reach a consensus on the main question/hypotheses for the manuscript. Normally, at least in our group, it requires several meetings, discussions, hard debates, etc, however, at the end, all authors should be happy with the main goals of the manuscript.

How do we develop those ideas/questions/hypotheses? To solve this problem, we designed the “QTNano Project Concept”, which is a set of statements that gives a QTNano paper its (i) motivation, (ii) justification, (iii) main goals, (iv) open questions, (v) methodology key points, (vi) task list, (vii) computational cost, (viii) risks, (ix) authors contribution statements, and (x) final remarks not addressed in the previous items. It is important to mention that the “QTNano Project concept”, as organized by the QTNano group is not a guarantee of successful, however, it helps to minimize a large number of problems along a master dissertation, PhD thesis, and postdoc project.

The QTNano project concept in computational physics, chemistry, and material science should has a maximum length of 2 up to 4 pages (hard cutoff) in double column format and must contains the following sections:

1. **Motivation** – writes one paragraph with a solid motivation to perform this work at this particular field, e.g., Can you visualize social and economical impact from this study?
2. **Justification** – writes one paragraph with a solid justification for the selected problem, e.g., why is so important to use our time and resources to solve this problem? Can we contribute to solve a real experimental problem? Is it an experimental-theoretical study? Did you talk with experimental groups about this problem?
3. **Main Goals** – writes a short paragraph (3 to 4 lines), in which you should summarize the main question/hypothesis/goal of this



Figure 5 Illustration diagram with all the key points of a project, which includes idea, execution, discussion of results, writing, risks, etc.

paper. If you cannot write this statement now, then, you are not ready to start this project, and further reading is necessary to improve your knowledge on this topic and identify a real important problem. From our conception, the supervisor can help to propose a problem, however, the group member must structure their ideas to enhance the goals, which requires a deep understanding of the literature, i.e., a good literature review is required. In case that you are not ready, then, improve your literature review once again using QTNano computational tools.

4. **Open Questions** – to reach your main goal, by sure, you need to answer several big/small questions. Here, you should list all your questions. A good paper propose to answer few questions and not too many questions, and hence, it is crucial to point out clearly the main question.
5. **Methodology Key Points** – summarize using a short paragraph the theoretical approach and computational details employed to reach your goals. Just list the name of the techniques, computational implementations, etc. You do not need to discuss computational parameters here, however, you can list few observations, which you might consider very important for all collaborators.
6. **Task List** – organize a list of tasks required to answer your questions using

the proposed methodology. The success of a particular paper depends strongly on the efficiency to set up a well defined list of tasks to reach our goals. Of course, the list of tasks should be revised as much as necessary in case that unexpected and unplanned situations take place.

7. **Computational Cost** – estimate the computational cost of this project based on the list of indicated tasks. For that, estimate the number of calculations (crucial), computational cost, and provide good expectations. Did you perform at least 5 calculations to evaluate the computational cost? Several projects faced very big challenges within the group because of misconceptions in the scaling of the computational cost by increasing the number of atoms.
8. **Risks** – indicate the risks in this project. Do you know all computational techniques and their minor details? Can you set up a proper force-field calculation in LAMMPS without mistake? Is the computational time higher or small comparative with different projects performed in the past? Do you have enough social skills to lead a manuscript with 10 authors? Do you have the technical skills to write an experimental-theoretical paper? Do you have writing skills to write a letter?

Do you have enough computational resources?

9. **Authors Contribution Statements** – list all authors and their role in the paper, e.g., project design, calculations, literature review, technical support, specific analyses, manuscript story-line, manuscript writing, manuscript revision, correspondent author, project supervision, obtaining grants, etc.
10. **Final Remarks** – summarize into a single paragraph your expectations for this paper, e.g., indicates a list of possible scientific Journals for publication, etc. At this document, we provide a list of possible journals, however, your suggestions should not be restricted by the our suggestions.

Thus, the project concept is a document composed by 10 sections, which has the aim to help the authors to drive their effort. From our experience, the initial effort employed to write the project concept pays off by reducing the time to develop the project and minimize problems among authors, etc. Furthermore, the QTNano project concept provides a solid training on the design and management of a project, which can help every group member in future.

6 Literature Review

Before starts our discussion, we should define the meaning of literature review. Basically, it is an overview of the previously published studies (technical reports, papers, books, etc) on a specific scientific topic. Nowadays, to perform a good literature review, we have to employ several search engines, which are required due to the large number of information, however, it is hard even hard to imagine a literature review without search engines, e.g., [Web of Science](#), Google Scholar, Science Finder, ResearchGate, etc. Therefore, a well done literature review requires solid training on some of those database platforms and good strategy minimize problems and maximize quality of the results.

At the QTNano group, we have worked along the years to improve the quality and speed of the literature review process, which can takes several steps with the aim to reach our goals with the highest quality, see Figure 6. Below, we

will discuss all the steps employed within the QTNano group.

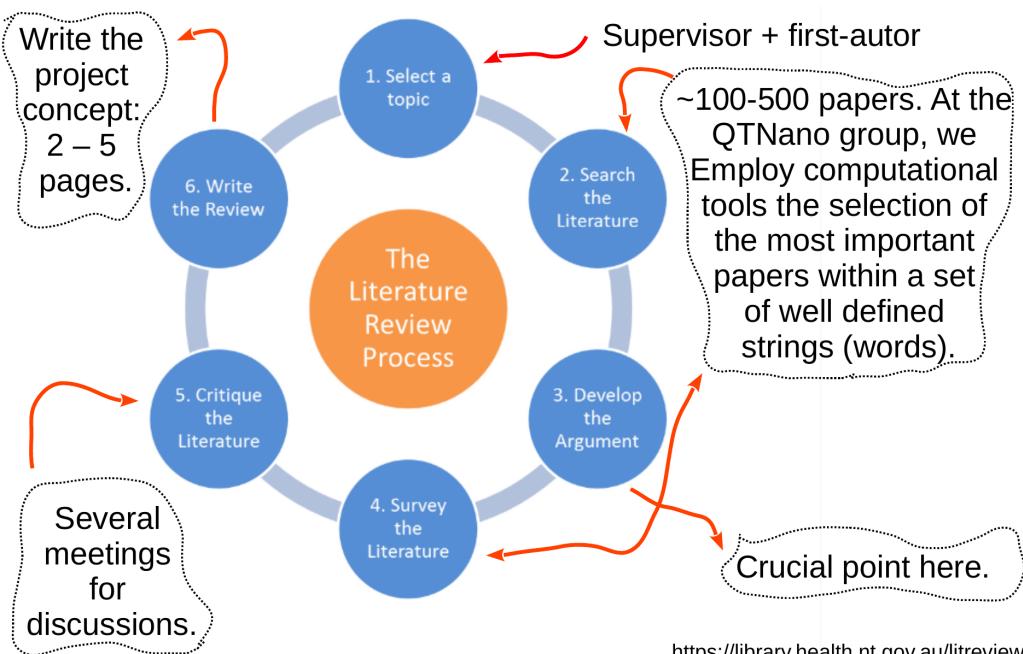
Select a Topic: A selection of a scientific topic can be done along with your supervisor/advisor. It is important to recognize that a good decision at this step will be great, however, in many cases the initial decision can be refined along the search of the literature, however, the task (literature review) will take longer.

Databases: Select one database or several databases, e.g., Google Scholar, Web of Science, Science Finder, ResearchGate, scientific journals, etc. We recommend to use a reliable databases, however, from our opinion, a proper training is one of the most important requirements. In case that you do not have a proper training on search engines, then, you need to ask for support for a QTNano group member.

Strings: Define a set of words (strings), which will be employed within the search engines of the online platforms. Thus, wrong strings imply on wrong literature search. Using good strings, we will obtain a very large number of papers, which can be organized by year period or by number of citations or even by the name of authors, etc, within the platform engines. Thus, at this point the number of available papers will be huge, i.e., in the order of thousands.

Select Papers: Based on the initial list of papers based on an initial set of strings, we can download a select number of papers (N_{papers}) based on several criteria, namely, number of citations, title, abstracts, authors, etc. Therefore, at this point, we will need to read only a fraction of the information available in the papers. At the end of this step, we will end up with about 500 up to 1000 papers easily or even more. Can we read every page of 500 papers? Yes, however, it takes a long time even reading one paper per day. For example, 365 papers will take 1 year in case that you read one paper per day.

Papers Hierarchical Classification: Thus, the literature review can be time consuming due to the size of the scientific literature, i.e., thousand and thousand papers are published each year. Therefore, we must employ computational tools to help to improve our productivity. At the QTNano group, we employed a script to build up a hierarchical classification of all papers (PDF files) based on the analysis of the full paper (PDF translated to text format). Our script is a simple implementation of the **Okapi BM25+** algorithm,



<https://library.health.nt.gov.au/litreview>

Figure 6 Schematic representation for literature review.

which ranks the papers based on the term frequency and document size employing up to 20 strings (words). To use our implementation of the Okapi BM25+ algorithm, we recommend to name all PDF files with the following names: **first-author-surname_page-number_year.pdf**.

Okapi BM25+ Algorithm: Basically, we convert all PDF files into text format, which can be analyzed easier than the PDF itself. Then, we select a set of up to 20 strings, and runs our script. Thus, at the end, we focus our effort (reading/studying) on a short selection of representative papers. Our tool is very simple, however, it provides a simple path to search thousands of PDF files at a single run, which takes a couple of minutes at the worst cases.* Thus, using a set of strings, it is possible to select the *most important* papers within the database, which improves and reduces time based on the organization of different directories, etc.

Nowadays, the literature follow up can be done using several complementary strategies:

1. Register at the most important scientific journals related with your research topic to receive the list of papers published in every edition. It is a great approach to follow up the literature, however, you should select only the most important journals at your field.

2. Register at the Google Scholar to receive the scientific publications of the most important researcher scholars at your research field. It provides a list of papers at your email every week.
3. An account at the ResearchGate can also help to follow the scientific literature, however, it requires additional time.

7 Practical Recommendations

Below, we provide several practical recommendations based on the QTNano experience, which will help to write your manuscript.

7.1 Language Support

All papers within the QTNano group are written in English as all papers are published in international journals published by American Chemical Society, American Physics Society, Royal Society of Chemistry, Elsevier, etc. We are not native English speakers, and hence, it is a challenge for most group members to write a scientific manuscript in English. However, from my own working experience, we cannot blame our difficulties to achieve excellence in scientific writing only on the lack of skills to write English at high level. As mentioned before, a paper reports a scientific work, which should

* The same scripts are also employed to search my PDF library, which contains about 10 thousand papers, and continues to grow year by year.

be done using several well defined procedures, rules, recommendations, computational tests, etc. Thus, logical organization of the scientific ideas is one the largest barriers to achieve excellence in scientific writing.

Below, we provide several recommendations to improve your skills in case that is necessary, however, if you are a native speaker this section will not help you too much.

1. Group members with difficulties to write in English should start a English course as soon as possible, and there is no exception for this recommendation. It will play a crucial role for your future career at the academic or outside it.
2. In case that you need additional support with correction of english sentences, etc, then, we recommend the following cloud english service platforms, www.writefull.com, www.trinka.ai, Grammarly, and etc, which provide free or premium license services.
3. Keep in mind that British and American English has few differences, which should be taken into account once the Journal is defined.
4. Overleaf highlight words with potential typo errors in several languages, and hence, it should be employed by all members.
5. In case that you are not using Overleaf, you can use aspell -c case.tex English corrector, i.e., a simple and efficient free software to remove typos.
6. We do not recommend to write the manuscript in your native Language, e.g., Portuguese, and translate to English using Google Translator. This procure will only delay your long term development.
7. At the QTNano group, we do not pay for English revision of the manuscripts.

7.2 Text Editor

At the QTNano group, we employ [Latex](#) as a tool to write all scientific documents, which includes scientific reports, papers, letters, undergraduate exams, master dissertations, PhD thesis, etc. Thus, our experience using Latex is broad, in

particular, because several tools and strategies were developed along the years to help our organization.

Therefore, all new QTNano members must learn Latex. Below, we provide the most important recommendations to use:

1. **Overleaf** – We recommended to use the LATEX version installed in the [Overleaf](#) platform, which is the official platform for writing documents at the QTNano group. Overleaf is described in Wikipedia as follows: *Overleaf is a collaborative cloud-based LaTeX editor used for writing, editing and publishing scientific documents. It partners with a wide range of scientific publishers to provide official journal LaTeX templates, and direct submission links. Overleaf was originally launched in 2012 as WriteLaTeX by the company WriteLaTeX Limited, co-founded by John Hammersley and John Lees-Miller. Both are mathematicians and were inspired by their own experiences in academia to create a better solution for collaborative scientific writing. They started developing WriteLaTeX from 2011. They launched the beta version of Overleaf on the January 16, 2014, at their first #FuturePub event held at the British Library in London. On the July 20, 2017, Overleaf acquired ShareLaTeX to create a combined community of over two million users. This led to the creation of Overleaf v2, combining original features from both into a single cloud-based platform hosted at overleaf.com. <https://en.wikipedia.org/wiki/Overleaf>.*
2. **Overleaf Errors** – Keep in mind that Overleaf does not show several minor errors in Latex, which can affect the submission of a scientific manuscript. Thus, always perform a cross-check compilation of your documents at your desktop before provide OK for submission. At the Overleaf, any document can be edited at the same time by all authors, which is the next level for collaborative scientific writing. Among several features of overleaf, **Track changes** and **Add comments** should be used as key features for any collaborative work.
3. **TexLive** – In case that you cannot use Overleaf, we recommend to use the TexLive installation at all QTNano

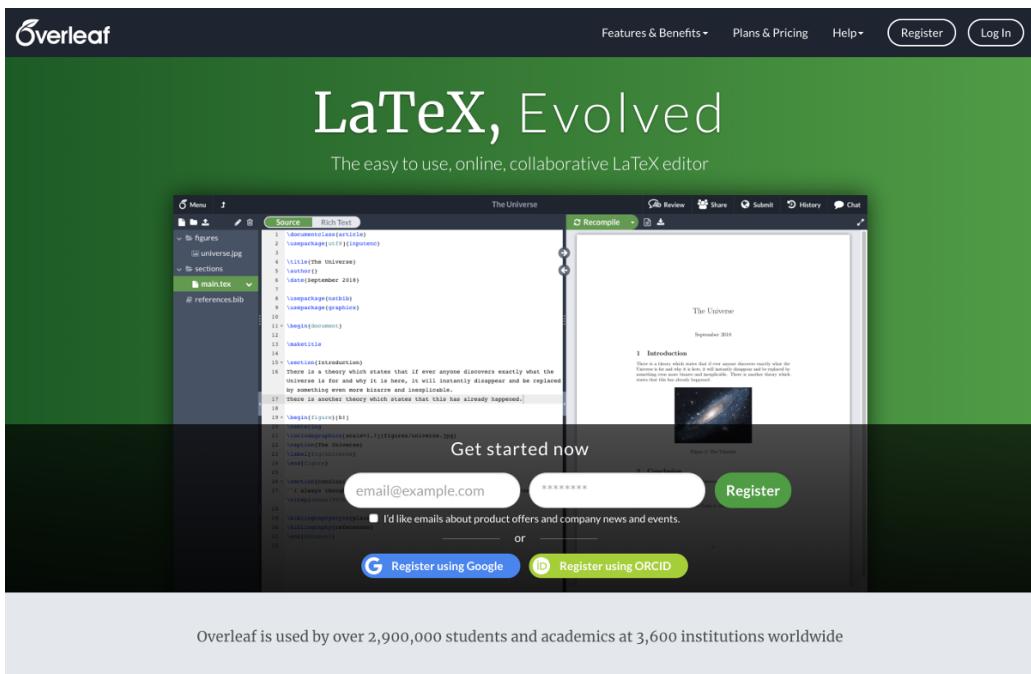


Figure 7 Overleaf login page. Nowadays, all scientific documents at the QTNNano group are written in the Overleaf Platform. Before Overleaf, we used TexLive at our own personal desktops.

Desktops (Ubuntu or Suse Operational System) at the São Carlos Institute of Chemistry, University of São Paulo. Furthermore, you have the option to use [MikTex](#) (Microsoft Windows).

4. **Latex Editors** – You can use several graphical Latex interfaces, e.g., TexMaker, TexStudio, etc. Furthermore, you can also use the traditional **vim** text editor, which is available in every Linux operational system.
5. **Obsolete Commands** – Please, do not use obsolete commands. Use the command **\RequirePackage[l2tabu,orthodox]{nag}** at the first line of your tex file. It helps to identify obsolete Latex commands, which should be avoided along the manuscript.
6. **Latex Class** – We should always use one of the following packages with their respective magazines standards. It is not hard to change from one format to another format, in particular, in case that all suggestions below are followed.
 - (a) **REVTEX**: American Physical Society format for manuscripts that will be submitted for APS journals. IoP magazines use also REVTEX.

- (b) **ACHEMSO**: American Chemical Society format for manuscripts that will be submitted for ACS journals. In case that the journal is defined yet, please, use the ACHEMSO template.
- (c) **RSC**: Royal Society of Chemistry format for manuscripts that will be submitted for RSC journals.

7. **Latex Chemical Equations** – All chemical formulas should be written with **usepackage[version=4]{mhchem}** and new versions of the package and **usepackage{siunitx}** beyond of all standard packages in latex.
8. **Latex New Commands** – We must avoid the definition of new commands within a manuscript as much as possible because it can create serious problems for compilation by the automatic procedures along the submission process at different Journals. Thus, we employ standard Latex commands and those provided by the packages.
9. **Latex Errors** – The first author has the task to solve every problem in compilation. All latex files should be compiled smoothly without any minor error. Keep in mind that the PDF files will be generated using automatic procedures along of the

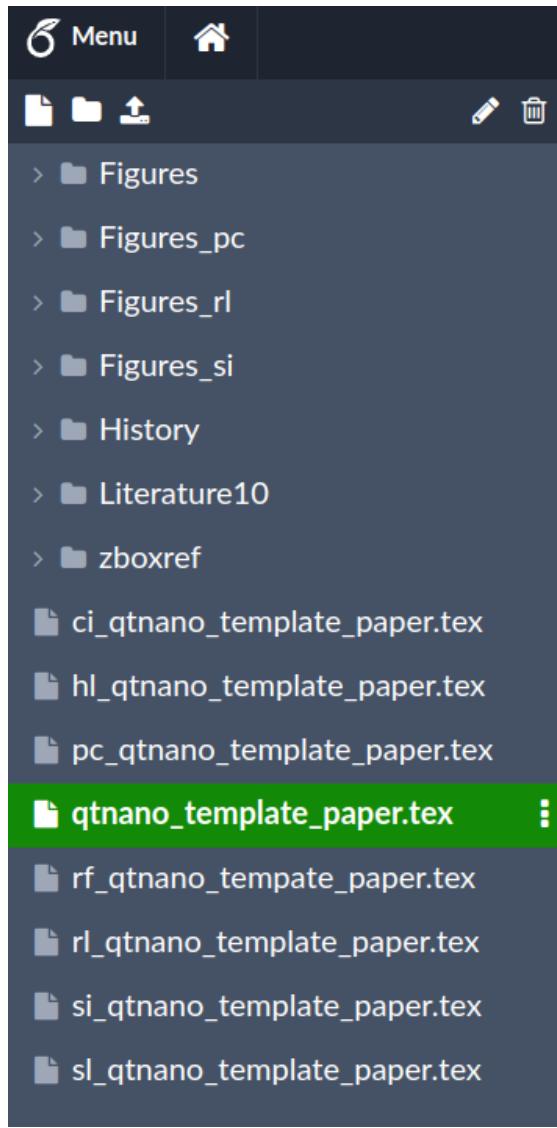


Figure 8 Manuscript files organization employed by the QTNano group at the Overleaf platform (template). The present file organization can be revised/updated based on group member suggestions or negative experience by the group members. We provided an updated template for every new manuscript once is required.

submission for few particular journals. For example, Latex files with problems cannot be compiled with success along the submission, and hence, the manuscript cannot be submitted. In case that all files are correct, a manuscript submission takes at maximum 30 minutes by Juarez L. F. Da Silva, however, with problems it can take hours or even days.

7.3 Files Organization

Once the Text Editor is selected (Latex), then, we should discuss the structural organization of directories, files, and so on, which is a critical step to minimize the time employed to write a good manuscript. At the QTNano group, we published several papers every year, and several manuscript are in progress at the same time by all group members and collaborators. In case that every one decides to define their own file structure, then, it would be a challenge for the group leader or collaborators to provide proper guidance for every one in short time because we will lost time to understand the organization of the files, etc.

New group members, in particular undergraduate and graduate students, have never written a scientific paper before, and hence, their organization skills are far behind the standards employed by advanced scientific writers, who have developed their skills for 20 years or even more. At the end of every year, as group leader, we revise all procedures employed by the group members with the aim to remove procedures that does work well any more, etc. For example, this file is revised every month with the aim to improve its structure, organization, and new ideas.

Thus, every member within the QTNano group should employ the same organization standards, Figure 8, which turns the life easier for everyone. Thus, using this procedure, a scientific initiation student (undergraduate student) will learn at early age all procedures employed by graduate, postdocs, an so on. Thus, it plays a crucial role in the communication flow among the group members and collaborators.

We employ the following directory structure for each manuscript within the Overleaf platform (www.overleaf.com) at the QTNano group:^{*}

1. **Figures** – directory that contains all figures that belongs to the scientific manuscript. It should includes only the final version of each Figure and it should not includes the figures employed for the electronic supporting information file. All figures for the manuscript should be in EPS format, which helps further edition by the editorial

^{*} The present structure is used by the QTNano group, however, it can be extended for different groups without too much problems as the those basic files are required for any manuscript submission.

production, etc. Overleaf is not a data repository, and hence, we should provide only the final figures and not all versions of the same figure.

2. **Figures_si** – directory that contains all figures that belongs to the electronic supporting information file. The number of figures can be very large at the electronic supporting information file, and hence, we recommend only PDF format for those files as those files will not be edited by the scientific journals (PDF files speed up Latex compilation). Keep only the final version of the Figures within this directory.
3. **Figures_pc** – directory that contains all figures that belongs to the project concept, i.e., manuscript road map. A flowchart can provide a great help in the project concept, and it should be allocated in this directory. All those Figures should be in PDF format.
4. **Figures_rl** – in case that is necessary, figures employed within the reply letter should located within this directory. All those figures should be in PDF format.
5. **zboxref** – directory that contains the reference bibtex files for the manuscript. We employ a very good structure for that, which helps everyone (see below) as each reference needs to be added only once by all group members. However, it is very important that every one follows the data structure organization and standards, which can be used by ACS, RSC, APS, IOP, etc.
6. **Literature10** – directory that contains the most important 10 papers related with this manuscript. It helps all readers to understand what are the main papers related with our goals. Those papers should be selected in the literature review. Of course, those papers are not related with the methodology.
7. **History** – a directory that contains history files, which are not useful any more, but the authors wish to keep by personal reasons.
8. **casemanuscriptfile.tex** – it is the the scientific manuscript file. Do not change the name of the file along of the manuscript preparation. Overleaf can keep history control at the state of the art, however, good training is required to use it properly.
9. **si_casemanuscriptfile.tex** – it is the electronic supporting information (ESI) file, which will be written along the development of the manuscript. At the QTNano group, we publish well documented ESI files within each publication.
10. **pc_casemanuscriptfile.tex** – it is the project concept (PC) file, which should has a maximum length from 2 up to 4 pages (double column format). It can be larger, however, it is not recommended and should be avoided. As discussed before, it contains the core/goals/etc of the manuscript.
11. **sl_casemanuscriptfile.tex** – it is the submission letter (SL) file.
12. **rl_casemanuscriptfile.tex** – it is the reply letter (RL), which has a specific format within the QTNano group to speed up the construction of the document by all authors.
13. **ci_casemanuscriptfile.tex** – it is a conflict of interest (CI) letter, which has required by particular journals.
14. **hl_casemanuscriptfile.tex** – it is a letter that summarizes the most important highlights (HL) reported within the manuscript, which has required by particular journals.
15. **sr_casemanuscriptfile.tex** – it is a letter that contains the list of suggested referees (SR), which has required by particular journals in separated document. Normally, all journals require a list of referee's suggestions within the online submission, while particular journals require a separated file with the suggestions.

At the first view, the present structure might look boring or old style or even non-productive, however, well defined procedures are crucial to reach solid goals, in particular, the training of human resources, e.g., undergraduate, graduate, and postdocs members.

7.4 Five Titles Rule

A scientific manuscript can reports an interesting result obtained from a straightforward study or a scientific achievement with far consequences for the humanity. In any case, the title should capture the correct message as mentioned in the previous sections. At the QTNano group, we recommend that all coauthors should provide five suggestions for the title based on their current understanding. This procedure has the goal to motivate everyone to think on the manuscript, which helps to identify the most important scientific achievements done along the study. Furthermore, it helps also to identify misleading conceptions among the authors, which can delay the outcome of the manuscript.

7.5 Figures

Figures are one of the most important parts of a scientific paper, in particular, because a well designed figure has the power to capture/translate complex concepts/ideas, which might require several text paragraphs to be explained for readers. Figures are about data representation, which can be take several forms, namely, bar graphs, frequency histograms, drawings, two- or three-dimensional plots, specific data representation employed in specific scientific fields, and graphical entries that summarize a complete new concept, etc.

From our opinion, several factors are crucial to design state-of-the-art Figures, which includes:

1. Deep understanding of the most important descriptors to characterize a particular problem. For example, two-dimensional band structures are employed to represent the electronic states (descriptors) from three-dimensional Brillouin zone in solids, i.e., it is like to take photos of the six faces of a cube and represent them on a two-dimensional ribbon (graphical representation).
2. Software for different type of data representation. For example, molecular representations require specific software, while two-dimensional graphics can be done with several tools.
3. Solid skills on graphical design and paper organization.

4. Furthermore, the following questions are important. What is the easiest figure representation of a physical-chemistry concept? Should we employ an schematic representation or real data representation to demonstrate a physical-chemistry concept?

Below, we will discuss several recommendations, which should be employed by all QTNano members.

Ethics: (i) All figures should contains only correct data. Furthermore, statistical error is required for particular studies, e.g., physical-chemistry properties derived from molecular dynamic simulations. (ii) No one can change the data reported in the figures, e.g., remove points or add new points to the graphics to improve agreement with experimental data. (iii) We cannot republish a figure from a previous paper from the QTNano group or someplace else as an original figure in a new paper.

Figure Data: All data used to build up figures should be available within the figure directories, e.g., the data used to build the `bulk_dos_1.eps` should be available within the `bulk_dos` directory. Furthermore, the data reported within a Figure should be reported within the electronic supporting information files.

software: The quality of a figure depends also the selected software, and hence, a good choose is important. Few recommendations based on the QTNano experience: (i) VESTA (open source) – recommended for molecular structure representations. Alternative software is possible, e.g., Crystal, Avogadro, Ovito, VMD, etc. (ii) `xmgrace` is an open source and strongly recommended software for two-dimensional plots.* In case that an author decided to use a different 2D graphics editor, then, he/she be aware that your software should be able to build up the same quality graphics as in `xmgrace` and good flexibility for changes, in case that is required at any time. (iii) Gnuplot for 2D and 3D plots, and so on. (iv) `xfig`. (v) Etc. (vi) We do not recommend Microsoft Excel to build up Figures for scientific papers at the QTNano group.

* It is called QtGrace for windows.

Quality: In particular for new QTNano members, do not try to build up the final version of the figures at the first trial. Initially, build up figures that captures the general idea, which should evolve in understanding and graphical design along the evolution of the manuscript. We recommend to discuss with the senior authors all results before build up your final Figures, i.e., a good figure should represent/translate a concept/idea. There are standard approaches to represent several results (properties) within the scientific community, and hence, study the designing of published figures within your group or literature papers for inspiration, Figure 9.

Figure Design: For single column figures (Figure 9), please, use A4 portrait size. In case that is not suitable, please, adjust that for your particular case. For double column Figures, please, use A4 landscape size. In case that is not suitable, please, adjust that for your particular case. Every figure should be color online and readable for black-white printers. This is very important. A figure must be re-done as many times is necessary to achieve this goal. Along the weeks, months, and years, you will improve your skills and be able to design and build up state-of-the-art figures at the first trial, which is recommended for every QTNano group member. Be patience, work hard, inspire yourself with previous papers, and so on.

File Format: Recommendation from *Science*, *It is best to create your figures as vector-based files such as those produced by Adobe Illustrator. Vector-based files will give us maximum flexibility for sizing your figures properly without losing resolution, as they can be altered in size while maintaining high print-quality resolution.* Therefore, at the QTNano group, we employ the following formats: (i) Encapsulated postScript (EPS) for manuscript figures, which are submitted along with the manuscript and the size within the paper will be adjusted by the editorial production. (ii) Portable document format (PDF) for all files figures within the supporting information file or different documents. It helps to speed up compilation within Overleaf and reduce file size. At the submission, we submit only the supporting information file, i.e., no separated figures are submitted. (iii) Different file formats will not be accepted for manuscript submission within the QTNano group.

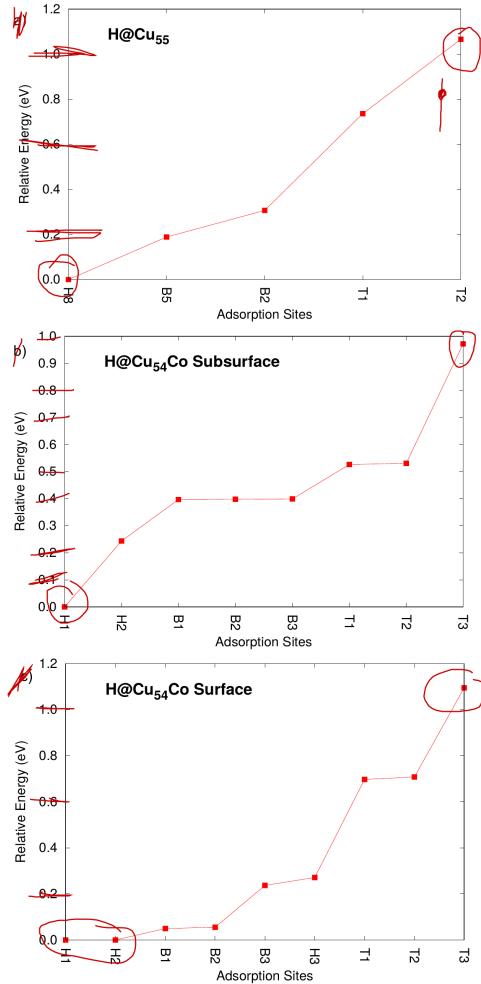


Figure 9 Example of figure with problems:
 (i) The size of the font employed for the numbers and axis labels are too much small compared with the text. (ii) There is a high-density of numbers in the *y*-axis graphics. (iii) The graphic legend is in bold, however, we recommend in standard text font. (iv) Several data points are located on the graphic frame as indicated by the circles. (v) The adsorption sites label should be written at the horizontal mode. (vi) We do not need to write Adsorption Sites for every graphic as the *x*-axis has the same meaning. We need only to keep the labels for the sites. (vii) We do not need to add a), b), and c) for the graphics as we provide a graphic legend for each graphic – double information.

File Size: For manuscripts (papers), we recommend only the EPS format, however, for particular cases such as molecular structures representation of several joined structures, the file size can be very large, e.g., 50 Mb or even 100 Mb. Thus, we recommend to use the *epstopdf* software (Linux) to change the format from EPS to PDF, which will have a smaller

size, e.g., up to 100 times smaller. Furthermore, in case that you need to reduce the file size of the PDF files even further, we recommend the following command: `gs -sDEVICE=pdfwrite -dCompatibilityLevel=1.6 -dPDFSETTINGS=/ebook -dNOPAUSE -dQUIET -dBATCH -sOutputFile=output "input.pdf"` or you can use a compact form of it, i.e., `gs -sDEVICE=pdfwrite -dPDFSETTINGS=/ebook -q -o output.pdf file.pdf`. At the end of the process, you should convert the file format to EPS. Nowadays, every figure should have a size of about 1 to 30 MB because particular scientific journals add a restriction to upload large files.

Figure Combinations: We should avoid combining 2 or 5 small figures within latex to build up a single figure. Each figure should be a single file. A figure composed by several small figures can create problems to perform the submission, as every figure file must be associated with only one figure number. There are several software that can be used to combine several figures in a single file, xfig, etc.

Figures Location: (i) All manuscript figures (EPS format) should be located in the **Figures** directory. Each individual figure should be located within a specific directory within the **Figures** directory with all the previous versions of the particular figure, at your computer (it does not apply within the Overleaf platform). Provides only the last version of the figure within the **Figures** directory in the Overleaf platform. (ii) All supporting information figures (PDF format) should be located within the **Figures_si**. (iii) Do not mix together in the same directory of the TEX files tons of figures or files. We have a well designed file structure for all papers. In case that you do not like it, do not cry, follow our recommendations and one day you might be a group leader and you will be able to define your own structure organization.

Figure File Names: All files should have a name that helps its identification easily along the development of the manuscript. Furthermore, it should not change along of the development of the manuscript. For example, the figure **bulk_dos_01.eps** should be located within the directory **bulk_dos** at your desktop. In case that we update the figure, then we change the name for **bulk_dos_02.eps**, and both figures located within the directory because we need to follow the development history of the present

manuscript. A bad designed figure today can be a good figure tomorrow and vice-versa. Please, never name your figures such as fig1.eps, fig2.eps, and fig3.eps, which does not help to revise the manuscript, etc. Figures can change their relative position within a manuscript and such names are useless to the organization. Only the final version of each figure should be uploaded to the cloud Overleaf platform.

Figure Label: Every Figure should have a label to be cited within the manuscript or supporting information using Latex. The name of the label should be the same as the name of the Figure, however, without the extension number, e.g., **fig:bulk_dos**, while the figure file name is **bulk_dos_02.eps**. It procedure helps to improve readability along revision process when you need to revise several papers at the same week, which is the case of several researchers.

Figure Caption: Figure captions should be succinct enough for the reader – explanation of results should not be included in the captions.

Recommendations by Prof. Prashant Kamat: Several short articles have been published with solid suggestions to improve the design of Figures for scientific papers, e.g., [Five Common Pitfalls to Avoid while Composing Scientific Figures](#) by Constance M. Biegel and Prashant V. Kamat, [Three Simple Ways to Identify Data Sets in a Figure](#) by Constance M. Biegel and Prashant V. Kamat, [Absolute, Arbitrary, Relative, or Normalized Scale? How to Get the Scale Right](#) by Prashant V. Kamat, [The Lost Art of Composing Single-Panel Figures](#) by Prashant V. Kamat, and [Ten Tips for Capturing Figures with Captions](#) by Constance M. Biegel and Prashant V. Kamat.

Furthermore, we summarize below several recommendations from [Science](#), which are important to prepare your Figures.

1. *From Keys to symbols, if needed, should be kept as simple as possible and be positioned so they do not needlessly enlarge the figure. Details can be put into the captions.*
2. *Use solid symbols for plotting data if possible (unless data overlap or there are multiple symbols). Size symbols so that they will be distinguishable when the figure is reduced. Line widths should be legible upon reduction (minimum of 0.5 pt at the final reduced size).*

3. Panels should be set close to each other, and common axis labels should not be repeated.
4. Scales or axes should not extend beyond the range of the data plotted.
5. Use scale bars in place of, or in addition to, magnifications. Do not use minor tick marks in scales or grid lines. Avoid using y-axis labels on the right that repeat those on the left.
6. Avoid using red and green together. Color blind individuals will not be able to read the figure.
7. Please do not use colors that are close in hue to identify different parts of a figure.
8. Avoid using grayscale.
9. Use white type and scale bars over darker areas of images.
10. Units should be metric and follow system international convention.
11. Use a sans-serif font whenever possible (we prefer Helvetica).
12. Simple solid or open symbols reduce well.
13. Label graphs on the ordinate and abscissa with the parameter or variable being measured, the units of measure in parentheses, and the scale. Scales with large or small numbers should be presented as powers of 10.
14. Avoid the use of light lines and screen shading. Instead, use black-and-white, hatched, and cross-hatched designs for emphasis.
15. Capitalize the first letter in a label only, not every word (and proper nouns, of course).
16. Units should be included in parentheses. Use system international notation. If there is room, write out variables – e.g., Pressure (MPa), Temperature (K).
17. Variables are always set in italics or as plain Greek letters (e.g., P , T , m). The rest of the text in the figure should be plain or bold text.
18. Type on top of color in a color figure should be in bold face. Avoid using color type.
19. When figures are assembled from multiple gels or micrographs, a line or space should indicate the border between two original images.
20. Use leading zeros on all decimals – e.g., 0.3, 0.55 – and only report significant digits.
21. Use capital letters for part labels in multipart figures – A, B, C, etc. These should be 9 pt and bold in the final figure. When possible, place part labels at the upper left-hand corner of each figure part; if a part is an image, set labels inside the perimeter so as not to waste space.

7.6 Tables

You will find Tables (one or more) in most scientific papers, which clearly indicates the importance of Tables for data representation within a scientific manuscript. Several authors think that it is possible to summarize all data using Tables within the manuscript along with scientific discussion of the most important results, however, it is not recommended because it is not easy to recognize trends and patterns from Tables compared with well designed Figures. Therefore, we should not overuse Tables in scientific manuscript.

We should use Tables within the manuscript only for the cases in which data representation via Figures does not work well or there is a special requirement, e.g., comparison between our data and previous published data (experimental or theoretical). For example, density of states, electronic band structures, molecular structures, electron densities, orbitals representation, etc, have been represented within papers via Figures, i.e., it is standard within the scientific community in computational material science.

As possible, all data employed for Figures within the manuscript should be reported within the Supporting Information using Table format. This approach cannot be applied easily for all cases, e.g., density of states Figure or band structures, however, it is recommended and should be implemented as possible. Unfortunately, you will not find the data employed for the Figures in most papers, in particular because electronic supporting information files is a new tradition.*

Below, we provide several practical recommendations and suggestions, which

* The same applies for public repositories, where crude data employed to write a scientific manuscript is provided for the scientific community, who can perform additional analyses to obtain new insights.

should be employed to improve the organization level of your manuscript:^{*}

1. Define clearly the data for Tables and Figures. We recommend to talk with all authors ahead to avoid lost time.
2. Define the Table size (number of columns and lines) based on the data, e.g., avoid tables with 2 columns or 2 lines. Furthermore, the number of columns or lines should not exceed the line width in the horizontal or vertical text size.
3. The caption should be well define, i.e., define all variables within the caption.
4. Do not change the font size to fit a Table within the width of the column/page size. This solution works for the moment, however, at the editorial process, the problem will rise up again. Thus, we need solid solutions for the manuscript organization.
5. We recommend the `siunitx` Latex package, which can provide great help to improve the quality of the table without the requirement to use `tablecolumn`, and so on. For that, we recommend to read the `siunitx` userguide (check the link – www.ctan.org).
6. Use the `longtable` package only if is really necessary because it affects Latex compilation time, etc, etc.
7. Do not use Table-Figure within a manuscript, i.e., a table composed by data and Figures at the same time, as it creates several challenges for submission. Every Figure file should be associated with a particular Figure.

7.7 Mathematical Notations

Normally, every researcher wish to define their own variables for the physical-chemical properties, e.g., ϕ or Φ or Ψ are commonly used for the wave function. Thus, it is common to find two or more papers from the same group using different notations or even misleading notations. Thus, to minimize this problem, we provide

^{*} A well organized manuscript will helps the spread of science as it can be read by less experience and advanced researchers.

several recommendations[†] below for the most common physical-chemical variables employed by the QTNNano group in their papers.

1. E_{tot} – Total energy.
2. E_{tot}^{DFT} – DFT total energy.
3. ΔE_{tot} – Relative total energy, which is defined using the following equation, $\Delta E_{tot} = E_{tot}^i - E_{tot}^{ref}$. Thus, as defined, the relative energy is the same as the total energy, however, using a selected energy (system) as reference (*ref*), e.g., *ref* = *lowest* for the lowest energy configuration.
4. E_{vib} – Vibrational energy contribution.
5. E_{vdW} – van der Waals energy contribution.
6. E_{ad} – Adsorption energy, where

$$E_{ad} = E_{tot}^{\text{CH}_4/\text{Cu}(111)} - E_{tot}^{\text{CH}_4} - E_{tot}^{\text{Cu}(111)}, \quad (1)$$

where E_{tot}^i indicate the total energy of the respective systems in the lowest energy configurations.

7. E_{int} – Interacting energy, where
8. E_{exc} – Excess energy, which is employed in the study of alloys.
9. E_{CBM} – Conduction band minimum (CBM) energy (selected among all \mathbf{k} -points within the Brillouin zone).
10. E_{VBM} – Valence band maximum (VBM) energy (selectex among all \mathbf{k} -points within the Brillouin zone).
11. E_g – fundamental energy bandgap calculated as the energy difference between the CBM and VBM energies considering all \mathbf{k} -points within the Brillouin zone, i.e., $E_g = E_{CBM} - E_{VBM}$. E_g can be a direct or indirect bandgap.

[†] All variables are defined in mathematical mode.

12. E_{CBM}^{Γ} – CBM at the Γ -point.
13. E_{VBM}^{Γ} – VBM at the Γ -point.
14. E_g^{Γ} – Fundamental energy bandgap calculated at the Γ -point, i.e., $E_g^{\Gamma} = E_{\text{CBM}}^{\Gamma} - E_{\text{VBM}}^{\Gamma}$.
15. $E_n^{\mathbf{k}}$ – Eigenvalue n at a particular \mathbf{k} -point.
16. E_{Fermi} – Fermi energy.
17. Φ – Work function, which is defined as the energy difference between the electrostatic potential at the vacuum level and the highest occupied state within the band structure, i.e., $\Phi = V(\mathbf{r}_{\text{vac}}) - E_{\text{Fermi}}$.
18. σ_s – Surface energy, which is calculated using the following equation,
- $$\sigma_s = \frac{1}{2}(E_{\text{tot}}^{\text{slab}} - N_l E_{\text{tot}}^{\text{bulk}}), \quad (3)$$
- where $E_{\text{tot}}^{\text{slab}}$ is the total energy of the 1×1 surface unit cell slab with N_l layers. $E_{\text{tot}}^{\text{bulk}}$ is the bulk total energy per atom.
19. $\sigma_s^{(hkl)}$ – Surface energy of the (hkl) surface, e.g., (111).
20. σ – Chemical order parameter.
21. m_{tot} – Total magnetic moment.
22. $m_{\text{loc}}^{\text{Ce}}$ – Local magnetic moment of the Ce atom.
23. $d^{\text{C-O}}$ – Bond length for the C–O bond.
24. V – Volume.
25. $\mathbf{a}, \mathbf{b}, \mathbf{c}$ – Lattice vectors in the Bravais lattice.
26. α, β, γ – Angles between the primitive lattice vectors in the Bravais lattice.
27. V_0 – Equilibrium volume.
28. a_0, b_0, c_0 – Equilibrium lattice parameters.
29. $\alpha_0, \beta_0, \gamma_0$ – Equilibrium angles between the primitive lattice vectors in the Bravais lattice.
30. d_0 – Ideal interlayer spacing distance (before surface relaxation); diatomic C–O molecule bond length, etc.
31. d_{ij} – Interlayer spacing upon relaxation of the surface atoms.
32. Δd_{ij} – Interlayer spacing relaxations, where
- $$\Delta d_{ij} = \frac{100(d_{ij} - d_0)}{d_0}. \quad (4)$$
33. ECN_w^i – Weighted effective coordination number given in number of nearest neighbours (NNN) for the atom i .
34. $\text{ECN}_{\text{av}}^{\text{Cu}}$ – Average weighted effective coordination number given in NNN for the Cu atoms.
35. ECN_{av} – Average weighted effective coordination number given in NNN.
36. d_w^i – Weighted bond length for the atom i .
37. $d_{\text{av}}^{\text{Cu}}$ – Average weighted bond lengths for the Cu atom, i.e., average over all Cu atoms.
38. d_{av} – Average weighted bond lengths for a selected system; average over all atoms.
39. $X_{\alpha}, Y_{\alpha}, Z_{\alpha}$ – Atomic coordinates of atom α .
40. \mathbf{R}_i – Vector indicating the position of atom i .
41. F_x, F_y, F_z – Atomic force components along the x -, y -, and z -directions, respectively.
42. \mathbf{F}_i – Atomic force (vector) on the atom i ; all vectors should be in bold.
43. Z_{α} – Atomic number of atom α .
44. Z_{val} – Number of valence electrons.
45. $Q_{\text{eff}}^{\text{Cu}}$ – Effective Bader charge on the Cu atom.
46. m_e – Electron mass.
47. M_{α} – Mass of atom α .
48. \hat{H} – Hamiltonian operator.

7.8 Reference Database

A good citation database is crucial to write a good scientific manuscript, thesis, reports, etc, and hence, special attention is required in this topic. Thus, it is natural to think on a database of references because several references are cited in

```

@Article{DaSilva_075424_2005,
  title = {\ce{Xe} Adsorption on Metal Surfaces: First-Principles Investigations},
  author = {Juarez L. F. Da{~}Silva and Catherine Stampfl and Matthias Scheffler},
  journal = {Phys. Rev. B},
  volume = {72},
  month = {Aug.},
  year = {2005},
  number = {7},
  pages = {075424},
  doi = {10.1103/physrevb.72.075424},
  url = {http://dx.doi.org/10.1103/PhysRevB.72.075424},
  publisher = {American Physical Society},
  timestamp = {2015.11.27},
  owner = {juarez}
}

```

Figure 10 Example of a single BibTex reference entry from our database file (`boxref_bibtex_DayMonthYear.bib`), which is maintained by Juarez L. F. Da Silva at the QTNano group. Today, 1 March 2022, our file contains about 4000 ready to use BibTex entries within the field of computational material science.

several papers, thesis, and so on. Furthermore, the same reference is cited by different group members. Therefore, at the QTNano group, we have employed a reference database using the Bibtex format, where all the entries are collected and organized at the same bib file (e.g., `boxref_bibtex_DayMonthYear.bib`) and used as needed by everyone. Our BibTex database entries contains all information (title, author, doi, journal, month, number, pages, publisher, url, volume, pages, year, issn, owner, timestamp, etc) required by all scientific journals, thesis, etc. Thus, it is easier to change from one submission at a particular journal from one publisher to another one using the same database.

As mentioned by [Overleaf](#), *when it comes to bibliography-management packages, there are three main options in LaTeX: BibTex, NatBib and BibLatex. BibLatex is a modern option for processing bibliography information, provides an easier and more flexible interface and a better language localization than the other two options.* However, at the QTNano group, we have used the old BibTex as it does the required job with good quality and has been employed by a wide range of publishers.

Below, we provide several recommendations:

1. Every one should use our `boxref_bibtex_DayMonthYear.bib`, which contains a large number of BibTex entries. The BibTtex entries are clearly organized, cross-checked, etc, which helps to make the life easier for every one within the QTNano group and collaborators.

2. To add new BibTex entries, you can use [JabRef](#),* [doi2bib](#), etc. Every new BibTex entry should contains all the fields, namely, title, author, doi, journal, month, number, pages, publisher, url, volume, pages, year, issn, owner, timestamp, etc.
3. In case that you do not wish to edit the `boxref_bibtex_DayMonthYear.bib` file, we recommend to build up your own boxref file, which you can name as `boxref_xxx.bib`. Both files can be included at the manuscript, and the BibTex will extract the required references from both files. We should not duplicate references between both files, which will affects Latex compilations.
4. Keys for the BibTex entries play a crucial role as several tools identify repeated BibTex entries based on the code keys. Thus, it is very important to use the same key definitions for all entries. At the QTNano group, we employ the following format for the BibTex entry namely,

* As defined in [wikipedia](#), *JabRef is an open-sourced, cross-platform citation and reference management software. It uses BibTeX and BibLaTeX as its native formats and is therefore typically used for LaTeX. The name JabRef stands for Java, Alver, Batada, Reference. The original version was released on November 29, 2003. JabRef provides an interface for editing BibTeX files, for importing data from online scientific databases, and for managing and searching BibTeX files. JabRef has been released under the terms of MIT license since version 3.6 (and was under the GPL license before). JabRef has a target audience of academics and many university libraries have written guides on its usage.*

First-author-last-name_page-number_year,
e.g., **Bittencourt_197656_2020**,
DaSilva_675656_2003, **Mendes_6787_2021**,
etc. In case of names with accents, the
accents should be removed to minimize
problems, i.e., the first-author last-name
should contains only alphabet letters.
Please, never employ code names such
as rf1, rf2, rf3, rf4, rf5, or something like
PerdewPBE2008.

5. The database file should be verified to make sure that all entries full fill all requirements by journal from all publishers, namely, ACS, RSC, APS, IOP, etc.
6. Keep in mind that ACS journals require paper title in upper case letters (following ACS standards) and initial and final page numbers. Make sure that those information are added properly for every reference to avoid problems at the end. In case that you are not sure, please, check our database for examples.
7. The author abbreviations should follow the standards employed in our database file, which works for all journals up to now, November 6, 2022.
8. Include DOI numbers in every BibTex entry. Nowadays, it is required by all publishers, and beyond of that, the paper can be recovered easily using DOI information.

Once every thing was done, then, we should organize the references for the manuscript submission. Do we submit the database for the journals? No, we do not do that. Basically, as mentioned above, we extract all references from the databases using the BibTex software, which generate a file called manuscript.bbl after Latex compilation. Thus, the following steps are employed:

1. latex case.tex or pdflatex case.tex.
2. bibtex case.aux.
3. latex case.tex or pdflatex case.tex.
4. Then, you obtain a case.bib file.
5. latex case.tex or pdflatex case.tex.

6. Just before the submission of the manuscript, the **case.bbl** file must be added at the end of the case.tex file, just before the latex command `\end{document}`. This procedure is very important as only a single TEX file with a separated file for each figure should be submitted for the journals. For example, you can use the command `cat case.bbl > case.tex`, and the problem will be solved.

7.9 Citation Procedures

Below, we provide several suggestions for citation procedures within the manuscript:

1. **How and when to use et al.** – The abbreviation “et al.” means “and others”, and it is widely used to shorten in-text author citations of papers with three or more authors. For papers with one author, then, cite the author last name, i.e., “AuthorOneLastName”, while for papers with two authors, we should write as follows: “AuthorOneLastName and AuthorTwoLastName”. Then, for papers with more than two authors, include the first author’s last name followed by “et al.”. We do not need to italicized “et al.”, as it is part of the enlgish language for centuries.
2. In case that 2 citations or more references are cited at the same point in the manuscript, we should follow a year sequence, e.g., `\cite{Rondina_678_1998, Sabino_56789_2000, Furtado_6789_2013}`. We should avoid citing a large number of papers at the end of the same sentence unless is really necessary, while the remaining of the manuscript does not contain citations. Citations are essential at the correct places and for the correct reasons.
3. Please, do not cite as the following example, `\cite{Rondina_678_1998}`
`\cite{Sabino_56789_2000}`
`\cite{Furtado_6789_2013}`, as it will affects the reference organization at the end.
4. We should avoid to cite url in papers, master or PhD theses because it requires additional work, e.g., you need to add the

access date for every cited url. We should cited www pages only in cases that we cannot provide a proper reference.

7.10 Acknowledgments

Today, November 6, 2022, our acknowledgments section at the QTNano group should be composed by all or few of the following statements:^{*}

1. **FAPESP-SHELL Project** – The authors gratefully acknowledge support from FAPESP (São Paulo Research Foundation, Grant Numbers 2017/11631-2, 2018/21401-7, NUMBER[†]), Shell and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&D levy regulation.
2. **CAPES** – This study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES) - Finance Code 001 (fellowships for NAME[‡]).
3. **CNPq** – This study was financed in part by the National Counsel of Technological and Scientific Development (fellowships for NAME[§]).
4. **Santos Dumont** – The authors acknowledge also the National Laboratory for Scientific Computing (LNCC/MCTI, Brazil) for providing HPC resources of the SDumont supercomputer, which have contributed to the research results reported within this paper. URL: <http://sdumont.lncc.br>.
5. **HPC LCCA USP and CETI-SC** – JLFD acknowledges the Advanced Scientific Computational Laboratory (University of São Paulo) and the infrastructure provided to our computer cluster by the São Carlos Center of Informatics, University of São Paulo.

Beyond of that, always as necessary, we should provide acknowledgment for technical support or scientific discussion for QTNano group members or external collaborators.

^{*} Those information should be updated every year.

[†] Replace NUMBER by an additional grant FAPESP number in case that is necessary. [‡] Replace NAME by the correct student name. [§] Replace NAME by the correct student name.

7.11 Authors Contribution Statement

Authors contribution statement is required by several journals, and hence, we should be prepared to provide this important information. Below, we provide an example:

1. **Author 1** – Methodology, software, formal analysis, investigation, data curation, writing original draft, visualization.
2. **Author 2** – Methodology, software, validation, formal analysis, investigation, writing review & editing.
3. **Author 3** – Formal analysis, writing review & editing.
4. **Author 4** – Formal analysis.
5. **Author 5** – Formal analysis, writing review & editing, supervision.
6. **Juarez L. F. Da Silva** – Conceptualization, methodology, resources, data curation, writing review & editing, visualization, supervision, project administration, funding acquisition.

For additional details on the role and term definitions, we recommend to check the link provided by [Elsevier](#).

8 Paper Writing Sequence

Every scientific group has their own culture and philosophy to write their scientific papers as it depends on the research area, data features, group size, etc. At the QTNano group, we provide the following sequence to write a manuscript in short time:

1. Write a transitory title, which is based on the initial discussions (project concept), however, it can evolves along the manuscript development. In principle, an accurate title at the first trial will speed up the process as it should contains the main message of the manuscript.
2. Provide the list of all authors and their sequence within the manuscript, and hence, it helps to provide the expectations on each author based on their position in the author list.

3. Methodology (Theoretical Approach and Computational Details). A well defined methodology helps to establish the remaining of the manuscript. Only the essential details are required at this section, which are required for data reproduction. Additional details should be reported within the electronic supporting information.
4. Figures – organize the initial figures, which should capture the main message of every important findings.
5. Tables. As mentioned above, we should not overuse Tables, and hence, it requires special care this task.
6. Results and Discussion – includes all subsections, etc. Furthermore, we recommend to write down a short sentence in each subsection with the main goals,, which will help to provide a direction for all authors.
7. Introduction or Conclusions. It is crucial to drive the introduction to the field, review the literature, point out the open questions, and provide your proposal to solve the problem or contribute to improve our scientific knowledge within the field.
8. Conclusions or Introduction.
9. Abstract.
10. Cross-check the Figures and Tables format.
11. Final Title.

9 Supporting Information File

The electronic supporting information (ESI) file* is a crucial and essential part of a good manuscript and widely employed by the QTNano group. It usually contains the following information in the field of computational materials science: (i) Computational convergence tests and additional technical details. (ii) Tables with data employed for the Figures within the manuscript, which

is really important for further comparisons. (iii) Figures using an alternative perspective or organization (energy range, size, etc). (iv) Complementary and non-essential discussions on the data. (v) Non-essential equations. (vi) Etc.

Normally, all those information are not included within the manuscript due to the limitation length, however, it is used as a peer-reviewed material by the Referees. Thus, it must be well organized, succinctly presented, and should contain only correct data. The length of the supporting information can extend from few to up 1000 pages, in particular, the number of pages can be very large once the atomic positions (molecular systems) can also be reported within the document. Below, we will discuss the most important sections required to the ESI file.

At the QTNano group, the ESI file provides solid complementary information for the manuscript. Furthermore, its construction is employed as a tool to follow up the development of all scientific papers within the group and with external collaborators. For example, along the development of a particular project (paper), all obtained data is included within the ESI, and shared with all authors via Overleaf (Cloud Platform) – a complete transparency for all authors. Once the study is completed, the QTNano electronic ESI file is separated into two parts, namely, (i) the most important results are transferred to the manuscript, (ii) while the complementary data remains as a ESI file for the manuscript. Thus, based on this procedure, the QTNano ESI file starts to be written at day zero and accessible for all authors via cloud platform. This procedure helps all QTNano members to organize their data since the first day, design good figures, tables, and so on. Therefore, all format, Latex, and so on mistakes can be corrected since the first day.

9.1 File Format

We should use single column file formats instead of the double column format employed for the manuscripts/papers.

9.2 Title

The ESI titles is the same as in the manuscript, however, preceded by the complementary **Electronic Supporting Information:** or

* The term *Supporting Information* is employed by scientific journals published by the American Chemical Society, however, the American Physical Society uses the term *Supplementary Material*, while the Royal Chemical Society journals uses the term *Electronic Supplementary Information*.

alternative definition based on the Journal recommendations.

9.3 Authors and Addresses

It should be exactly the same as in the manuscript.

9.4 Authors Email

At the QTNano group, we recommend that all authors provide their emails at the ESI file. For fresh graduate and postdocs members, we recommend to use their personal emails as their professional emails will change often at this stage of the career. Therefore, based on this procedure, any reader can contact all authors of the paper in case that is necessary.

9.5 Computational Details

In computational materials science, we should report all computational details for data reproduction, however, it is not possible to provide all data within the manuscript. Thus, at this section, we should report additional computational details required for data reproduction by interested readers, e.g., list of PAW projectors, basis functions, INPUT files, etc.

9.6 Computational Tests

To characterize material properties within the field of computational materials science, we employ computational techniques to solve quantum chemistry equations using approximate methods. Therefore, our results depends on the computational parameters employed for those simulations. Then, it is recommend that at least the most important computational parameters should be tested for the selected systems, and the data should be reported within the ESI file. It helps further readers to understand our procedures and data reproduction in future.

9.7 Additional Figures and Tables

Additional Figures and Tables can be provided within the ESI file, which can help any reader. For example, the data of a Figure or graphic can be reported within the ESI as a Table, in particular, for important data employed for

comparison with experimental results. Several times, compact figures are provided within the manuscript, while separate figures with additional details can be provided within the ESI file or different scale, e.g., energy or length scale. The Figures and Tables should have good quality as in the manuscript. For the size of the Figures within the ESI file or manuscript, we recommend to use `width=0.80\linewidth`.

9.8 Molecular Structures

A molecular structure plays a crucial role in atomistic computational physics, chemistry, and material science, as the atomic positions (x, y, z) of every atom within a molecular structure are employed as input for atomistic simulations, e.g., *ab initio* quantum-chemistry, molecular dynamics, etc. Thus, in case that a reader or even the referee wish to reproduce the results within a given paper, it will be impossible without the correct molecular structures. Therefore, for every published paper, we report the most important employed molecular structures using recommended formats n separated files or even within the PDF file in text format.

Our procedures has been recognized as “Excellent Science Practices” by several referees, and hence, we keep our standards, which is also recommended by the scientific community. Furthermore, a cross-check of our results is also welcome, as accidental mistakes can occur even using a large number of procedures to avoid that. For large number of molecular structures or crude data, we recommend to use public data repositories to archive your data, which should be accessible for every one. For a long list of specific or generalist repositories, see the link [Data Repository Guidance](#), which summarizes a long list of public or paid repositories. Furthermore, see our discussion on the Data Management Plan, Section ??.

9.9 File Organization

The data within the ESI file should be organized following the same sequence as in the manuscript file, and not as a historical sequence of the work and analysis performed along the project. In case that need, at the end of the preparation of the manuscript, the authors should re-organize the ESI file by re-order the sections, etc. Furthermore, along the manuscript

discussion, citations should be provided for the ESI file with the correct names, e.g., Figure 25S.

9.10 Page Numbering

The pages should be numbered by S-*i*, where *i* is the page number. Tables and Figures should be numbered as Figure S*j*, where *j* is the number of the Figure. This procedures can be done automatically using Latex (see the QTNNano templates).

includes theoretical/computational data or experimental data, i.e., a good literature review is always necessary. A good and recommended practice is the reproduction of previous published data by well established scientific groups or previous data from the group. In case that your data does not agree with previous studies, then, it is a sign that something might be wrong or unclear. All efforts should be done to understand and solve all those discrepancies.

10 Recommendations for Data Quality

Good science is based on good data, which requires well defined tools, procedures, metrics, and scientific analysis to be obtained. Several studies take years of data collections, which can extend up to 50 years in some fields of science, however, in most cases, the scientific work must be completed from 2 up to 4 years, which is the standard time for master and PhD programs world wide.

10.1 General Remarks

Below, we provide several recommendations based on our experience, which can help to improve the quality of the data:

1. The experimental or computational procedures employed to obtain your data should be revised several times with all collaborators (paper co-authors) or with colleagues with solid expertise working in the same field.
2. Any sign of error or strange behavior within the experimental or theoretical data should be investigated deeply with all co-authors to understand and obtain a solid solution for the problems. The identification of such problems is simple, however, the lack of experience or too much self-confidence of fresh graduate students play a critical role at this point. Thus, from our perspective, a correct supervision and follow up by all collaborators (paper co-authors) is essential to minimize all those problems.
3. All data should be compared with the literature as much as possible, which

4. All results should checked and cross-checked several times before publication. In case that a group member do not do the job properly, and we find problems just before the submission process of a manuscript or even a PhD thesis, the calculations must be re-done or re-organized or extra calculations must be done to complete the data. It is very important and we should take it very serious.
5. In case that a wrong result is published, an erratum should be published to correct the problem as soon as possible.
6. In case that a group member fake a set of data by his/her own will, then an investigation will take place by the senior group members. In case that a problem is confirmed, then the group member will leave the group at the next day without the rights to continue the same project at a different group.

10.2 Computational Remarks

In computational physics, chemistry, and material science, the following specific recommendations can be applied:

1. Is the physical-chemistry model reliable to answer all proposed questions written within the project concept? Several projects fails at this point, which is discovered after several months of scientific work. By analogy, the foundation of your new home is not solid to support the weight of your swimming pool at the second floor.
2. Is the theoretical framework reliable to provide a solid and accurate description

- of the calculated physical-chemistry properties? This is a common mistake in several manuscripts, which affects their acceptance, and hence, the work must be redone.
3. Did you check the convergence of the computational parameters? The lack of well defined computational parameters that yield well converged results is a very common problem within fresh graduate students.
 4. Did you check your input files with experts in the field?

5. Do you have a proper training in the field of the selected problem?
6. Are you able to separate a wrong simulation from a correct simulation? In case that you are not, then, you are not prepared to perform this project without close supervision.

11 Academic Integrity

Every one in the scientific community can summarizes several cases of failure in academic integrity, which includes a wide range of problems that goes beyond plagiarism* in projects, master dissertation, PhD thesis, and papers. Below, we separate and discuss the procedures employed by the QTNano group to improve academic integrity.

11.1 Procedures for Data Quality Control

1. All data employed to write a scientific paper should be available for all authors at any moment along the development of the scientific work.
2. All co-authors are in charge for checking the quality and procedures employed to obtain all data.

* According to Wikipedia, *plagiarism is the representation of another author's language, thoughts, ideas, or expressions as one's own original work. In educational contexts, there are differing definitions of plagiarism depending on the institution. Plagiarism is considered a violation of academic integrity and a breach of journalistic ethics. It is subject to sanctions such as penalties, suspension, expulsion from school or work, substantial fines and even incarceration.*

3. The procedures to obtain the data should be discussed with all authors and transparent for every one, which includes detailed information within the electronic supporting information file, e.g., all parameters should be reported, additional data not discussed in the manuscript, etc.
4. At the QTNano group, the electronic supporting information file starts to be written together with the simulations and not at the end of the scientific work. This file is an important tool to follow up all scientific work at the QTNano group.

11.2 Plagiarism Software: Turnitin

All documents written within the QTNano group, e.g., master dissertations, PhD thesis, articles, technical reports, etc, are cross-checked for plagiarism using the software [Turnitin](#) (online platform),[†] which identify similarities between the source document (PDF format) and a huge database of documents. Due to the large number of manuscripts in progress at the same time at the QTNano group, it is impossible to keep track of every piece of information, and hence, software like [Turnitin](#) is necessary as a supporting tool for scientific writing. For example, an author writes few or even several papers per year using computational tools, which parts of manuscript is employed as template to write a second manuscript and so on. Thus, tools like [Turnitin](#) can help to identify those type of mistakes, which every one wish to avoid because those are non-intentional plagiarism can also affect our scientific reputation.

11.3 Actions in Case of Academic Misconduct

The following actions are taken in case of academic misconduct:

1. In case that non-intentional errors are identified in computational simulations/calculations, then, the first author or the author in charge of the simulations/calculations (experiments) should repeat every thing again to solve

[†] The Turnitin license is provided by the University of São Paulo free of charge for all faculty members.

Turnitin Originality Report: Example

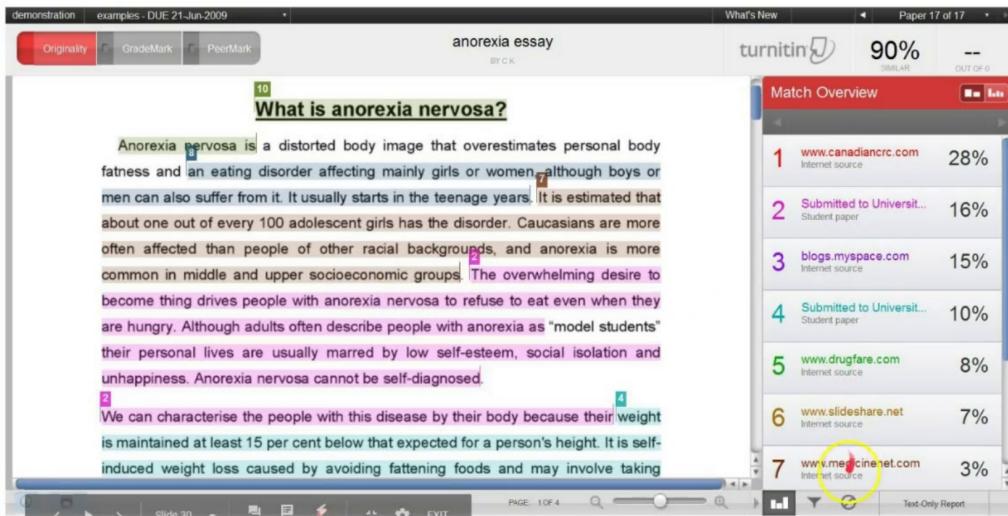


Figure 11 Example of the application of the Turnitin software at a random manuscript to illustrate its real life application.

the problems. We wish to avoid those situations, however, they happen by several different reasons. In most cases, it implies that some of the authors of the work in progress failed to perform their work (cross-check input files, supervision, etc).

2. Every identified error should be communicated to the leading author as soon as possible to discuss the following up procedures.
3. The cover up of non-intentional errors in computational simulations are the same as intentional errors, and hence, we apply zero tolerance for those situations once the problems are identified.
4. In case that of intentional errors in the calculations (e.g., lower cutoff energies to speed up simulations/calculations), data manipulation, cover up of mistakes, etc, are identified in the calculations (experiments), then, the group member will be asked to leave the group for good. At the QTNano group, we apply zero tolerance with academic misconduct of his members or collaborators.
5. In case that non-intentional plagiarism are identified within the manuscript, then the authors should revise the manuscript as soon as possible. In most cases,

non-intentional plagiarism are related with previous published papers from the manuscript authors due to the use of previous manuscript as templates, and so on.

6. Intentional plagiarism from previous work is a very serious infringement, which cannot be accepted. In such cases, which includes identical copy of information (full paragraph, sections, etc) from previous publications, the group member will be asked to leave the group for good.

12 Scientific Journals

Nowadays, there are tons of scientific journals, and every year several new journals are launched within the scientific community. Furthermore, we are going through a crucial transition, i.e., the journals are moving from permitted access paid by the readers (libraries) to open access, in which the publication charges are paid by the authors. Thus, graduate or fresh postdocs face great challenges to prospect for good journals to publish their scientific studies. Even though that is not clear for fresh researchers, the correct choice has far consequences for your scientific career, i.e., number of readers of your paper, which affects the number of citations and a possible stable job in future. Below, we will summarize important remarks, which can help in your decisions.

12.1 Journal Selection – Jane Support

At the end of every scientific study, every one expects to obtain a well written and solid scientific manuscript, which will be submitted for consideration for a selected scientific journal. In case that you do not have no idea or hint to pick up a good scientific journal, we recommend to use JANE platform, <http://jane.biosemantics.org/>, which can provide several journal suggestions based on the analysis of the title and/or manuscript abstract. Thus, the authors can use the present journals list to select few journals as possible candidates for the submission. This procedure is relatively very good for the cases in which you are starting a new project, or when you are not familiar with the most important journals in that particular field. Do not pick up the first journal in the list, as additional factors should be taken into account for the final choose, which will be discussed below.

12.2 Journal Impact Factors

Everyone wish to publish their scientific work at the most prestigious scientific journals such as Nature, Science, Journal of American Chemical Society, Physical Review Letters, etc, which are measured by the magnitude of the journal impact factors (JIFs). As defined in Wikipedia, *the JIF of an academic journal is a scientometric index calculated by Clarivate that reflects the yearly mean number of citations of articles published in the last two years in a given journal, as indexed by Clarivate's Web of Science. As a journal-level metric, it is frequently used as a proxy for the relative importance of a journal within its field; journals with higher impact factor values are given status of being more important, or carry more prestige in their respective fields, than those with lower values. While frequently used by universities and funding bodies to decide on promotion and research proposals, it has recently come under attack for distorting good scientific practices.*

Thus, you might be one of the researchers that hate the JIF parameter as we cannot measure the impact/quality of a research study based entirely on a single parameter such as the JIFs, however, it is a simple and intuitive descriptor for everyone. Furthermore, there is no alternative descriptor to replace JIFs, however, it is possible to employ additional scientometric parameters, e.g., *h*-index, number of citations,

etc, to balance those analyses. Further, it is a discussion that is far beyond the scope of the present white paper.

As everyone knows, there are several natural and unnatural barriers to publish at the highest quality journals such as Nature, Science, Journal of American Chemical Society, Physical Review Letters, etc, namely, (i) the originality of the scientific work; (ii) the quality of the scientific contribution and its social and economic impact for our modern life; (iii) beyond of that, the quality of the presentation is crucial nowadays, as mentioned and discussed by Prof. Dr. Prashant Kamat (Webinar at the CINE channel at the Youtube); (iv) additional factors, which we are not aware yet.

12.3 Recommendations

As expected, at the QTNano group, we have worked to improve the quality of our publications year by year, which requires substantial resources and human efforts. At the QTNano group, the training obtained by the undergraduate or graduate student along the development and writing of a scientific manuscript is more important than the JIFs itself. Thus, we should be caution on the selection of our goals, i.e., the goal is not high JIFs at all cost. Therefore, the main goal is the publication of high quality studies, which can be recognized by the international community as keystone results, and hence, be cited by the national and international scientific communities.

The QTNano group is composed by undergraduate (scientific initiation) and graduate (master and PhD) students, which are in the group to obtain high quality education, as well as postdocs members. Thus, the expectations are different on each group based on their scientific experience and fellowships values, e.g., a FAPESP fellowship is about 10 times higher than an undergraduate FAPESP fellowship. Thus, it is fair to expect higher scientific contributions from postdocs. Furthermore, from the QTNano perspective, it is very important that all QTNano members can publish their studies in scientific journals, which includes also undergraduate students.

Therefore, at the moment, November 6, 2022, we recommend the following expectations (minimum): all publications should be submitted for journals with impact factor

higher than 8.0 (postdocs), 5.0 (PhD students),^{*} 4.0 (master students),[†] 3.0 (undergraduate students).[‡] The JIF recommendations are only for guideline purpose, however, it works also as expectations for all group members, which is important in any group. Table 1 summarizes the most common journals for our publications (successful publications).

13 Suggestions of Reviewers

Most of scientific journals require suggestions of potential peer reviewers (name, email, professional address, and etc), which should be provided by the correspondent author at the manuscript submission process. At most journals, the submission procedure cannot continue without those suggestions, however, from our knowledge, several scientific journals do not apply this requirement. In any case, it is important to mention the following, i.e., it is the editor's responsibility to choose the reviewers among the suggested ones or pick up alternative names, who can be anonymous or disclosed by the journal. In the computational physics, chemistry, and material science community, several of the scientific journals recommend or require the suggestions of peer reviewers, and hence, we should be prepared to provide these suggestions at the submission procedure. At the QTNano group, we have organized a list of unbiased suggestions for peer reviewers along the years based on the following criteria:

1. Co-authors of our previous papers, even that it was published 20 years ago, should not be considered.
2. We do not recommend reviewers located at the same academic institution or a nearby friend of one of the authors in the present manuscript.

* At the QTNano group, we require 3 papers as first author for a graduate student to conclude his/her PhD thesis. Furthermore, the PhD student can collaborate in about 3 papers along his/her PhD program. † At the QTNano group, we require at least one paper from a master student to conclude his/her master dissertation. ‡ It is not a rule that an undergraduate student can publish a paper as a first author, however, several of our undergraduate students have achieved this goal. From our experience, it takes about 2 years for an undergraduate student to publish a paper with the support from a graduate student.

3. For each manuscript submission, we recommend to include potential peer reviewers from different continents.
4. We suggest only reviewers with several publications within the field or related to the study reported within the respective manuscript, i.e., we should consider only experts in the field.
5. At the QTNano group, we suggest reviewers with *h*-index higher than 40, which is a controversial suggestion, however, it has the goal to improve the quality of the scientific reports, which can contribute to improve the quality of the manuscript at the end.

14 Author Checklist Before Submission

This section was suggested by Prof. Dr. Prashant Kamat, who reads the present document on November 1, 2022 (personal communication). Based on his suggestion and inspired by a set of remarks reported within the link [ACS Energy Letters Author Checklist](#), we organized an author checklist, which should be verified before the submission of every manuscript. Our author checklist is summarized below:

1. **Title 1** – The title should be the same at the manuscript, supporting information, submission letter, etc.
2. **Title 2** – The manuscript title should be written in title case (ACS standards) or using different journal standards (Elsevier), etc. In general, we recommend to use ACS format for all manuscripts.
3. **Author List** – All authors names and email addresses should be provided correctly within the manuscript, supporting information, submission letter, etc.
4. **Table of Contents Graphic** – A table of Contents (TOC) graphic should be provided for every manuscript submission. The image size should follows the descriptions provided by the selected journal.
5. **Abstract Size** – Please, check if your abstract follows the journal requirements,

Table 1 Our publications within the QTNano group or in collaboration with different scientific groups are published in the following journals (black color) along with their journal impact factors (JIFs > 5.0). Furthermore, the publishers (American Chemical Society – ACS, Royal Society of Chemistry – RSC, American Physical Society – APS, Elsevier, etc) are also indicated at the first column.

Publisher	Journal Name	JIFs 2020	JIFs 2021
Elsevier	Applied Catalysis B: Environmental	19.503	24.319
Wiley-VCH	Angewandte Chemie International Edition	15.336	16.823
RSC	Journal of Materials Chemistry A	12.732	14.511
ACS	ACS Catalysis	13.084	13.7
ACS	ACS Applied Materials & Interfaces	9.229	10.383
APS	Physical Review Letters	9.161	9.185
Elsevier	Journal of Catalysis	7.920	8.047
Elsevier	Fuel	6.609	8.035
Elsevier	Applied Surface Science	6.707	7.392
ACS	ACS Applied Energy Materials	6.024	6.959
ACS	Journal of Physical Chemistry Letters	6.475	6.888
IOP	2D Materials	7.103	6.861
Elsevier	Journal of Molecular Liquids	6.165	6.633
RSC	Catalysis Science and Technology	6.119	6.177
ACS	Journal of Chemical Information and Modeling	4.956	6.162
Elsevier	Flachem	5.227	5.829
ACS	Inorganic Chemistry	5.165	5.436
RSC	Dalton Transactions	4.390	4.569
ACS	ACS Applied Electronic Materials	3.314	4.494
ACS	Langmuir	3.882	4.331
IOP	Journal of Chemical Physics	3.488	4.304
ACS	Journal of Physical Chemistry C	4.126	4.177
Elsevier	Journal of Luminescence	3.599	4.171
RSC	RSC Advances	3.361	4.036
APS	Physical Review Materials	3.989	3.980
AIP	Applied Physics Letters	3.791	3.971
RSC	Physical Chemistry Chemical Physics	3.676	3.945
APS	Physical Review B	4.036	3.908
Elsevier	Computational Materials Science	3.300	3.572
ACS	Journal of Physical Chemistry B	2.991	3.466
Springer	Journal of Cluster Science	3.061	3.447
Elsevier	Physica E	3.382	3.369
ACS	Journal of Physical Chemistry A	2.781	2.944
IOP	Journal of Physics: Condensed Matter	2.333	2.745
Elsevier	Surface Science	1.942	2.070
RSC	Materials Advances	0.000	0.000

i.e., several journals provide a maximum number of characters or words.

6. **Figures and Tables** – Check all Figures and Tables before submission, in particular, font size, quality, file size, size of tables, captions, etc.

7. **Notes** – Include conflict of interest information, if required by the journal.
8. **Check** – Cross-check the acknowledgment section of the manuscript, in particular, grant numbers, etc.
9. **References** – Check that all references have the authors name, correct journals

Manuscript Number: JCOU-D-21-00350

Ab initio Study of CO₂ Activation on
Pristine and Fe-decorated WS₂ Nanoflakes

Dear Prof. Dr. Da Silva,

Thank you for submitting your manuscript to Journal of CO₂ Utilization. After careful evaluation, I regret to inform you that your manuscript is not suitable for publication in the journal, and I must therefore reject it.

For alternative journals that may be more suitable for your manuscript, please refer to our Journal Finder (<http://journalfinder.elsevier.com>).

We appreciate you submitting your manuscript to Journal of CO₂ Utilization and thank you for giving us the opportunity to consider your work.

Figure 12 Example of a direct manuscript rejection by the Editor (received by email). A paper can be rejected by several reasons, and hence, do not give up, however, you should improve your manuscript before a new submission.

abbreviation, page number or electronic identify number, volume number, etc. Furthermore, several journals also require the title too.

10. **Latex Compilation** – All scientific manuscripts are written within the Overleaf platform, which employs Latex text editor. Of course, all files should be compiled without errors within Overleaf or at your desktop (Texlive) before submission.

15 Peer Review

Commonly, submitted manuscripts are evaluated by a peer review process, which has the goal to assess the quality of a manuscript before its publication by a particular scientific journal.

15.1 Editor Evaluation

The first evaluation is done by the Journal Editors, who are in charge to perform the quality assessment of a particular submitted manuscript. Upon the initial evaluation, Editors should take

the decision to send the manuscript for peer review process or reject it directly based on his initial evaluation. Normally, authors receive Editors decision within days or weeks, however, particular journals can take longer. Negative decisions are provided by email (faster), while the positive decisions (send for peer review) are commonly updated in the journal platform submission system, i.e., from “with editors” to “with referees”.

This step is a challenge, in particular, for high impact-factor journals, where the rate of success to cross the editor evaluation is very narrow. For example, it can be one digit in percentage at the highest impact-factor journals such as **Nature** – 9.8 % in 2005 - 7.6 % in 2017. Unfortunately, it is almost impossible to argue with an editor decision.

As pointed out by **Nature**, several criteria are employed by the Editors to send a manuscript for peer review or not:

1. *Report original scientific research (the main results and conclusions must not have been published or submitted elsewhere).*
2. *Are of outstanding scientific importance?*
3. *Reach a conclusion of interest to an interdisciplinary readership.*

Therefore, it is very important to write a manuscript that delivers the correct message, i.e., scientific writing plays a crucial role here. We can question the criteria employed by each journal Editor, however, at the end, there are only two possible answers, i.e., YES or NO.

Suppose that you followed up all document recommendations, however, at the end of the process, you received a negative report such as in Figure 12. The impact of the final answer can be different for different persons. For example, a fresh graduate student at his first or second papers, who is not familiar with the procedures, might be very frustrated, while a senior researcher is familiar with those unsuccessful cases. At the end, there are two possible routes: (i) Select a new journal for a fresh submission; (ii) Take the opportunity to revise the manuscript, improve manuscript preparation, figures, tables, captions, etc, and then, select a new journal for a fresh submission. At the QTNano group, we recommend the second option.

15.2 Rejection Based on the Referee Reports

Suppose that the manuscript was send to the peer review process by the editors, and hence, few reports will be received by the Editors within a time window. Based on the peer review reports, the Editors can take two possible paths: (*i*) Reject the manuscript directly or (*ii*) recommend publication with major revision, minor revision, or even publication as is it.

15.3 Recommendation for Publication

As mentioned above, a recommendation for publication might requires additional work, in particular, for major revisions of the manuscript, which is the main reason to write this section. A correct evaluation of the report is critical for the success publication of your manuscript as an incorrect evaluation of the report can drive you to the wrong path, in particular, it can happen for fresh researchers.

For example, a PhD student works for about one year doing his/her scientific research (experiments, etc) and additional few months to write the manuscript. Thus, after a long and intense work, most of the authors are not prepared to receive critics and negative comments on their work, and wrong reactions can affect the approach to write a good and well balanced reply letter. Furthermore, the approach to write the reply letter will also affects the procedures to improve the quality of the manuscript.

15.4 Writing the Reply Letter

From our understanding, the first evaluation of the report should be done by the leading author of the manuscript, e.g., corresponding author, who should point out the most important questions and indicates the challenges to write the reply letter and highlights the most important points to be addressed in the revised manuscript. Thus, from our opinion, the leading author should separate the referee reports in several questions to provide a clear and straight path to write the reply letter. At the QTNano group, this work is done by the group leader or leading collaborators.

Thus, the following steps are employed to write the reply letter at the QTNano group:

1. Separate the referee reports in several questions. Thus, the separation of the report into several questions is a crucial step for the success of the reply letter. Normally, this task should be done by the corresponding author.
2. The first author should read every question and provide his/her answer, which should be revised by all remaining authors.
3. Once all the questions are answered by the first author, then, the first author should revise the manuscript accordingly and consistently with the reply letter. Thus, the manuscript should be revised by all authors.
4. At this step – it is critical to take the opportunity to improve Tables, Figures, and additional changes in the text if necessary or indicated by the authors. We should improve the manuscript as much as possible before its final approval for publication.

15.5 Marked Manuscript

All editors and referees request the marked manuscript version, which helps to evaluate the changes performed by the authors within the revised manuscript. The construction of a marked manuscript is not a simple task to be done manually, as it requires a huge effort to indicate in red (removed text) and blue (new text) along the full manuscript. All those changes are required based on the referee comments, suggestions, critics, as well as based on the authors ambition to improve the manuscript even further. Several times, we have found that coauthors avoid to improve the manuscript because of the hard work required to build up the marked manuscript, i.e., they assumed that everything was hand made.

At the QTNano group, we employ the `latexdiff` software to build up the marked manuscript, Figure 14, which employs the old and the revised manuscript (new) versions to obtain the marked manuscript. Once the `TEX` file marked manuscript is generated, then, it can be compiled by `Latex`, which yields a marked `PDF` file for submission. The compilation of a marked `TEX` file can be a challenge, in particular, errors with marked Tables, and so on.

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Dear Editor

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Journal of Chemical Information and Modeling

Thank you for considering our manuscript for publication as a regular article. We have considered all the reviewers critics and suggestions in this revised version of the manuscript. Below, we address every comment and provide a summary of the changes made in the manuscript and supporting information. Furthermore, we added also the marked manuscript, where blue indicates new text and red indicated removed text.

1. **Reviewer 1:** This paper reports an original computational approach based on a machine learning algorithm to study an old problem, the structural changes induced in small transition metal clusters by the adsorption of CO molecules.

Authors: We thank the Referee for the careful reading of our manuscript. As mentioned by Referee, our work employs machine learning techniques for structure design and analysis; however, it is also worth mentioning, the use of Density Functional Theory (DFT) calculations as the main tool to address the effects induced by the adsorption of CO molecules on the structure of 13-atom clusters. We have taken into account the comments of the Referee and improved the current version of the manuscript.

2. **Reviewer 1:** The authors have performed a throughout analysis of the structural changes induced on M13 clusters by the addition of a growing number of CO molecules and have analyzed the origin of the structural modification using an energy decomposition approach.

Authors: We thank the Referee for the careful reading of our manuscript.

3. **Reviewer 1:** Before the paper can be recommended for publication, a number of issues, mainly related to work previously done on this subject, must be addressed.

Authors: We thank the Referee for the valuable comments/suggestions to our manuscript once all the remarks are properly addressed.

4. **Reviewer 1:** On a technical side, the ground state of Pd13, Rh13, Ru13 etc clusters is magnetic (see e.g. Moseler, M., Hädkkinen, H., Barnett, R. N., Landman, U. (2001). Structure and magnetism of neutral and anionic palladium clusters. Physical review letters, 86(12), 2545; Reddy, B. V., Nayak, S. K., Khanna, S. N., Rao, B. K., Jena, P. (1999). Electronic structure and magnetism of Rhn ($n=2\text{Å}\pm 13$) clusters. Physical

Review B, 59(7), 5214; Kaiming, D., Jinlong, Y., Chuanyun, X., Kelin, W. (1996). Electronic properties and magnetism of ruthenium clusters. Physical Review B, 54(3), 2191), but here it seems that spin polarization has not been taken into account. While this is probably not going to change the general conclusions, it certainly changes some aspects of the study.

Authors: First of all, we are grateful for the recommended references. All calculations were performed with spin polarization, as mentioned in Section 2.1 "Total Energy Calculations". Now, in the new version of the manuscript, we have improved and highlighted this aspect of spin polarization (in Section 2.1), citing the references suggested by Referee, as well as we have included the magnetic moments results, which improve our discussion.

5. **Reviewer 1:** The fact that CO adsorption changes the structure of metal clusters has been studied with electronic structure methods also before, see e.g. McKenna, K. P., Shluger, A. L. (2007). Shaping the morphology of gold nanoparticles by CO adsorption. The Journal of Physical Chemistry C, 111(51), 18848-18852; a reference is in order.

Authors: We thank the Referee for the suggested reference, which was appropriately cited within the manuscript.

6. **Reviewer 1:** Along the same line, the quenching of magnetic moments induced by CO on Ni clusters has been demonstrated long before the study of ref. 13 (see e.g. van Leeuwen, D. A., Van Ruitenbeek, J. M., De Jongh, L. J., Ceriotti, A., Pacchioni, G., Hådbergen, O. D., Rätsch, N. (1994). Quenching of magnetic moments by ligand-metal interactions in nanosized magnetic metal clusters. Physical review letters, 73(10), 1432; Pacchioni, G., Roesch, N. (1995). Carbonylated nickel clusters: from molecules to metals. Accounts of chemical research, 28(9), 390-397). Also in this case a proper reference is desirable.

Authors: We thank the Referee for the relevant references, which were properly cited within the revised version of the manuscript.

7. **Reviewer 1:** Finally, an aspect that is never mentioned is that of temperature. The fact that metal cluster carbonyls have a fluxional behavior at room temperature is known since decades (see e.g. Benfield, R. E., Johnson, B. F. (1981). Structures and fluxional behaviour of transition metal cluster carbonyls. Transition Metal Chemistry, 6(3), 131-144; Farrugia, L. J. (1997). Dynamics and fluxionality in metal carbonyl clusters: some old and new problems. Journal of the Chemical Society, Dalton Transactions, (11), 1783-1792). Can the authors discuss the role that temperature could have on the transformation of one structure into another one?

Authors: The study of the dynamics and fluxionality in transition-metal clusters is a hot topic at the moment, in particular, due to the importance of single-atom catalysts, in which the changes in the structure are crucial. Thus, the present question

Figure 13 Example of the format of the reply letter employed by the QTNano group.

Furthermore, the present software can be used by the leading author to check and verify if all the request changes were in fact implemented by the remaining authors of the manuscript. Thus, using the `latexdiff` software, the marked manuscript can be obtained in few seconds before submission. Therefore, it is an exceptional tool (`latexdiff`) with multiple functions within the QTNano group.

16 Proof Reading

Finally, after several months or years of hard work, the manuscript is accepted for publication by a journal. Thus, it is time for celebration with all coauthors, however, the job is not finished yet. At the end, we should approve the paper proof version, which is the paper version edited by the journal editorial production office. Normally, once the manuscript is approved, the manuscript is moved in the production line to the journal editorial production office, which will perform several actions on the manuscript, namely, (i)

revise the language at a certain level, which includes even re-writing misleading sentences, (ii) reduce or increase figures, (iii) format the final version of the manuscript, and (iv) etc.

The editorial revision is done at the highest level, however, mistakes can be introduced along the revision, e.g., changes meV to MeV, which affects the magnitude of a number and changes completely the meaning of the sentence. Furthermore, although the authors have done a great job, mistakes such as typos were missed in the previous revisions. Thus, it is an opportunity to revise the manuscript for the last time. Thus, the revision of the proof is the last opportunity to improve the manuscript, and every author should perform their task.

Normally, the editorial office will provide a list of queries, which should be revised by the authors. Beyond of that, all authors should read the manuscript to remove possible typos, which can compromise the take home message.

induce changes in the geometry–electronic structure, relative stability, and catalytic properties, structure, electronic properties, and relative stability in comparison with original gas-phase systems.^{3,4} Therefore, along the years, several studies have been reported with the aim to improve our atomistic understanding of the physical-chemical parameters that drives those changes. As show below, our knowledge has improved by several studies, however, our comprehension—as we will summarize below, our atom-level understanding is still unsatisfactory as there is no framework to identify those mechanisms for general cases.

As exemplified by Yudanov *et al.*⁵ using density functional theory (DFT) calculations for CO adsorption on Pd_n clusters, $n=13-116$, they showed that the magnitude of the CO adsorption varies with the size particle, i.e., starting in large particles with surface structure composed by close-packed facets, the CO bonds get weaker to the size of dozens of atoms. On the other hand, for small clusters the fraction energy changes as a function of particle size, which is expected due to the quantum-size effects, while the higher number of low-coordinated atoms is higher, providing a higher activity for CO adsorption and, consequently, higher in small clusters contributes to enhance the CO–Pd_n interactions. In the same line, using hybrid DFT calculations, Okunura *et al.*⁶ suggested that the surface of Au nanoclusters form active sites for catalytic reactions, because of the charge polarization in Au nanoclusters interacting with CO molecules.

Guedes-Sobrinho *et al.*⁷ investigated, via DFT calculations, the effects of high-coverage CO adsorption on the structural, energetic, and electronic properties of (Pt_nCo_{95-n}) Pt_nCo_{95-n} nanoalloys, where they found a shift in the stability towards higher Co composition upon the CO adsorption. This finding was explained by a decreasing in stress release as a consequence of smaller magnitude for the attractive Coulomb energy between the anionic surface and the cationic core region, i.e., the CO-adsorption affects the anionic charge in_{in} McKenna and Shluger,⁸ using a combination of

DFT calculations and thermodynamic models, verified the morphological transformation of Au₇₉ nanoclusters upon interacting with a CO atmosphere at low pressure and room temperature, which was explained by the strong dependence of the adsorption energy on the low-coordinated Au sites on the surface.

Based on DFT calculations and *ab initio* molecular dynamics simulations, Austin *et al.*⁹ investigated the behavior of the CO/Au₁₃ systems using the several structural models, namely, *I*_h, *O*_h, and planarsymmetries for Au₁₃. They found a 2D to 3D structural transition relative stability change, where 3D clusters can accommodate more charge on the core than 2D clusters due to CO interaction. Furthermore, Morrow *et al.*¹⁰ investigated the effects of CO adsorption on 13-atom PtAu clusters at different compositions and hence, as expected, they obtained that CO binds preferentially on Pt sites due to the partially occupied Pt *d*-states, which facilitates the hybridization of the Pt *d*- and CO-states.

In addition to studies on the CO adsorption effects on noble metal clusters, Fielicke *et al.*^{11,12} have performed experimental studies based on vibrational spectroscopy on the CO interaction with early and late TM clusters from 3 to more than 20 atoms, considering the dependence of the CO frequency with size and charge of the cluster and comparing with CO adsorbed on extended surfaces. For example, emphasis is given to the study for the size- and charge-dependence for CO adsorption on Co, Rh, and Ni clusters,¹² as well as, on Ni, Pt, and Pd.¹³ Furthermore, from Stern-Gerlach magnetic deflection measurements, it is demonstrated that the CO adsorption on Ni_n clusters ($n=8-18$) reduces the magnetic moment, similar to the magnetization quenching effects of CO on both Ni nanoparticles–Ni systems (nanoparticles, clusters, and thin films).¹⁴⁻¹⁶

Thus, as mentioned above, there is no general scheme to address the mechanisms that drive the relative stability changes due to the adsorption of molecular species on clusters. Thereby, using DFT within van der Waals corrections, we

investigate the relative stability change in the TM₁₃ clusters induced by the adsorption of *n* CO molecules, where TM = Ru, Rh, Pd, Ag, and $n=1, 2, \dots, 12$ ($n=1-6$). Based on those calculations, we proposed a general scheme to perform an energy decomposition of the binding energy of the *n* CO/TM₁₃ systems, which is used to identify the driven-mechanism-for-most important energy contributions that drive the relative stability changes due to the adsorption of molecular species. Our scheme is general, and it can help to improve our understanding in different studies.

2 Theoretical Approach and Computational Details

2.1 Total Energy Calculations

Our calculations are based on spin-polarized DFT within the semilocal formulation generalized gradient approximation¹⁷ proposed by Perdew–Burke–Ernzerhof¹⁸ (PBE) for the exchange-correlation energy functional.¹⁸ To , which can provide an accurate description of the structure,¹⁹ energetic,²⁰ electronic,²¹ and magnetic^{22,23} properties of the selected 13-atom clusters. Furthermore, to improve the description of the CO–TM₁₃ interactions, we employed the van der Waals (vdW) semiempirical D3 correction proposed by S. Grimme.²⁴ To solve the Kohn–Sham equations, we employed the all-electron Projector Augmented Wave^{25,26} (PAW) method, as implemented in the Vienna *Ab initio* Simulation Package (VASP),^{27,28} version 5.4.1.

For the unprotected Ru₁₃, Rh₁₃, Pd₁₃, and Ag₁₃ clusters in gas-phase, we employed the following cutoff energies: 361 eV, 278 eV, 282 eV 361, 278, 282, and 281 eV, respectively, which are larger by 12.5% than the recommended cutoff energy, i.e., the ENMAX parameter within the POTCAR files. For the *n* CO/TM₁₃ calculations, we employed a cutoff energy of 450 eV due to the presence of the C and O atoms,

which requires higher cutoff energies than the studied TM species.

To minimize the interaction between the clusters–finite-size systems and their periodic images, we employed cubic boxes with size of 17 Å (TM₁₃) and 22 Å (*n* CO/TM₁₃), which yield a minimum distance of about 12 Å among between the systems and its images. The Brillouin zone (BZ) integration was performed using only the Γ-point as there is no dispersion in the electronic states within BZ. For all calculations, the equilibrium geometries were reached once the atomic forces are smaller than 0.025 eV/Å on each atom and using a total energy convergence of 1.0×10^{-5} eV.

2.2 Representative TM₁₃ Configurations via the k-means Clustering Algorithm

To obtain a set of representative structures for Ru₁₃, Rh₁₃, Pd₁₃, and Ag₁₃, we selected about 65 optimized structures for each TM₁₃ system-cluster from previous DFT-PBE calculations.^{19,29} All those structures were re-optimized using the DFT-PBE+D3 framework –and, except for Rh₁₃ (see discussion below), the addition of the vdW D3 correction does not change the pGMCs for those the selected TM₁₃ clusters. For the *n* CO-adsorption study To investigate the relative stability of the *n* CO/TM₁₃ systems, we selected 5 representative TM₁₃ structures among the 65 optimized structures for each system, Figure 1, for which we employed an unsupervised machine learning algorithm; named the *k*-means clustering algorithm.³⁰

The *k*-means algorithm divides the dataset (clusters) into *k* groups of similar objects(feature—vectors).³¹ Hence, it is necessary to provide *k*. Thus, for its application, *k*-means requires as input an encoded representation of the TM₁₃ clusters for the *k*-means algorithm(feature vectors) and the number of groups, *k*. In this work, the feature vectors for each individual cluster are composed of the eigenvalues of the Coulomb

Figure 14 Example of a marked manuscript obtained by the difference of two TEX files (old and new versions) using the `latexdiff` software. It is an essential computational tool for manuscript re-submission at the QTNano group.

17 Conclusions

The present document is a *in-progress* document, which is often revised by the author. It summarizes the most important procedures employed within the QTNano group at the São Carlos Institute of Chemistry, University of São Paulo, and should be employed by all QTNano members. This technical document is also available from the Researchgate, and hence, it can be distributed freely for your colleagues in different groups.

References

- Kamat, P. V. Five Key Attributes of an Effective Title. *ACS Energy Lett.* **2021**, *6*, 1857–1858, DOI: 10.1021/acsenergylett.1c00755.