REVIEWERS' COMMENTS:

Reviewer #1 (Remarks to the Author):

A Framework for Putting Scientists' Eyes on Glass-Box Physics Rule Learner and Its Application to Nano-Scale Phenomena

The manuscript presents an interesting perspective on the use of ML in physical sciences. They introduce a concept called convolved information index and a corresponding linking function to identify the mathematical expressions in the underlying processes, providing glimpses to the ML+Physics with superior interpretability. I found the manuscript well written and the authors have shown satisfactory numerical results to demonstrate their approach for an array of applications in nano-scale CE phenomena. The paper is well presented and contains information and guidelines that are not easily found in the open literature. Moreover, I believe that the results presented here will be interesting for researchers dealing with ML/AI applications in transport processes as well as domain scientists in other areas. Therefore, I recommend the publication of this manuscript.

Reviewer #2 (Remarks to the Author):

The manuscript deals with the application of machine learning algorithms to unveil relations for physical problems. The manuscript is very well written, the theory well presented (although more details would be welcome) and the examples demonstrative. The problem addressed is interesting and shows that the proposed procedure is promising. It is an open question, but for further research, to see if the procedure applies to many other problems, and whether they may be combined with gray-box modeling (i.e. when some part of the physics are well known).
The manuscript is of high scientific quality, so in summary, in my opinion, the manuscript may be accepted in its present form.

**Responses to Editor's Comments**

The authors would like to express sincere gratitude for the comments and suggestions from the editor. They turned out to be highly constructive and instrumental for improving the quality of this research outcome. The authors thoroughly revised the manuscript to best comply with the constructive feedback.

Detailed responses to individual comments are presented in what follows. Original comments are given in bold blue letter while the authors' responses are given in black letter. The corresponding changes are copied herein in the bracket for editor' convenience.

**Please either approve the editor's summary or provide a suitably revised version. (see below). For further details please refer to the accompanying email.**
**"Using machine learning to interpret complex, multistep experimental process and reveal otherwise unknown physical rules is a field that is still in development. Here, the authors design a convolved information index and a corresponding link function in order to identify mathematical expressions with the underlying physical processes of nanoscale contact electrification."**

- Responses: The authors appreicate the editor's draft of research summary. The authors suggest to use the following summary:

  "Using machine learning to interpret complex phenomena and reveal unknown physical rules is an active research frontier. Here, the authors address how to combine basic physics, a convolved information index, and a transparent flexible link function to identify mathematical expressions of the underlying physical processes of nanoscale contact electrification."

**"*Manuscript titles are to be a maximum of 15 words. Please edit the title so it fits within this word limit.**
***In addition, this title does not read well. Is the term 'scientists' eyes' a technical term widely used in the community? I would recommend this is removed from both the title and abstract and kept to the introduction where it can be properly elaborated on.."**

- Responses: The authors agree with the editor's suggestion. The new title read as:

  "A Framework for Glass-Box Physics Rule Learner and Its Application to Nano-Scale Phenomena"

  Also, we removed "scientists' eyes" from the Abstract too.

**"Please be careful not to overstate the novelty/importance of your results. All results published in Communications Physics are novel and present a significant advance. We therefore prefer that such language is avoided in individual articles."**

- Responses: The authors agree with the editor's suggestion. Throughout the paper, the "novel" is removed accordingly.

**"The abstract must be less than 150 words and accessible. It should include the background and context of the work, 'Here we show' or an equivalent phrase, and then the major results and conclusions of the paper. It must not contain references."**

- Responses: The new abstract is less than 150 words and has been revised to follow the editor's suggestion.

**"To comply with our article templates, the text must be split into:**
**- Introduction (<1000 words), which must include the background and rationale for the work. The final paragraph should be a brief summary of the major results and conclusions. The results of the current study should only be discussed in this final paragraph. The Introduction should contain no references to figures or tables.**
**- Results, which must be split into subheaded sections, ensuring that the subheadings are no longer than 60 characters including spaces. Subheadings should contain no punctuation.**
**- Discussion, without subheadings.**
**- Methods, which must be split into subheaded sections, ensuring that the subheadings are no longer than 60 characters including spaces."**

- Responses: The authors revised the Introduction (<1000 words) such that first paragraphs present the background and rarionales for this work whereas the last paragraph presents a brief summary of the major results of the proposed work.

- Response: The authors changed the Conclusion section to Discussion without subheadings, and also added Methods section followed by subheaded subsections. Detailed methods and proposed algorithms are moved to this Methods section.

- All subheadings are less than 60 characters (with spaces).

**"at its burgeoning state -> It is not clear what you would like to say here. Do you mean 'in its infancy'?."**

- Responses: The authors revised the statement to a more clear explanation as

  [But, the extension of deep learning to 3D data sets is an active research area facing many theoretical and computational challenges]

**"Although advanced machine learning (ML) methods gradually conquer and innovate the hitherto human-dominant actions**
**-> The use of words such as 'conquer' and 'human-dominant' are types of words less appropriate for a scientific manuscript. Please replace such words with less dramatic adjectives."**

- Responses: The authors appreciate the edior's suggestion. We revised the statement to a more scientific expression as:

  [Although advanced machine learning (ML) methods gradually master and replace the complex actions that require the human-level intelligence and control capabilities]

**"It is still in its infancy for ML to learn real-world physical experimental data featured with three-dimensional (3D) objects and multifaceted physical measurements**
**-> This sentence is difficult to read and I recommend restructuring."**

- Responses: The authors appreciate the edior's opinion. We restructured the statement to a more clear expression as:

  [A direct adoption of an advanced ML method can rarely guarantee successful learning and prediction of the real-world experimental data that often contain three-dimensional (3D) objects and multifaceted physical measurements.]

**"In particular, we propose a framework that can facilely deal with multifaceted measurements of 3D specimens, infuse basic physics principles and scientists knowledge, extract hidden rules with transparent expressions, and evolve the rules with increasing data through the Bayesian update scheme**
**-> This sentence is difficult to follow. Please restructure.**

- Responses: The authors agree with the edior's opinion. We broke down and restructured the statement to more clear expressions as:

  [In particular, we propose a framework that can facilely deal with multifaceted measurements of 3D specimens by incorporating basic physics and scientists' experience. Also, the framework can extract hidden rules in terms of transparent expressions which will evolve with increasing data through the Bayesian update scheme.]

**"Still, this study differs from prior works in several aspects: this framework focuses on transparent expressions of hidden physics rules by leveraging scientists' basic experiences and knowledge, not relying upon the predefined global governing equations; this framework is built upon two novel ingredients, externalized multilayer "convolved information index" and "link functions" which in essence re-interpret and inherit the deep learning's successful philosophies; the identified expressions can evolve by embracing other physics rules; this framework is purely data-driven, requiring no distributional assumptions about priors and posteriors compared to (14)**
**-> This sentence is far too long and should be broken in order for it to be easier to read."**

- Responses: The authors agree with the edior's opinion. We broke down and restructured the statement to more clear statements as:

  [Still, this study differs from prior works in several aspects. First, this framework focuses on obtaining transparent expressions of hidden physical rules. Second, it seeks to leverage basic physics and scientists' experience rather than relying upon the predefined global governing equations. Third, it is built upon two ingredients, the externalized multi-layer convolved information index and flexible link functions which reinterpret and inherit

the deep learning's successful philosophies. Last, the identified expressions can easily evolve by embracing other physics and more experience. In essence, this framework is purely data-driven, requiring no distributional assumptions about priors and posteriors compared to (14).]

**"Please make sure that figure are referenced in order. Fig. 1 e appears to have been cited before Fig. 1b-d. If necessary please relabel the figure."**

- Responses: The authors changed all figures' labels in order cited in the text.

**"Please make sure that references have been cited in order. It would appear that ref. 19 has been cited before 16-18."**

- Responses: The authors rearranged all references as they are cited in the text.

**"* Please make sure to submit all figures separately as editable, high-resolution files in vectorgraphics format (.pdf, .eps, .ai etc but not .jpg, .bmp, .tif etc)**
*** Ensure all figures are cited in order in the text.**
*** All figures should have a title briefly describing the whole figure. Titles should not contain punctuation and should not cite figure panels.**
*** Figure titles should be brief, and ideally no longer than about one line, with minimal symbols. Please shorten this title, moving any details to the start of the caption.**
*** Each x- and y-axis should be individually labelled.**
*** Remove scale bar labels (keeping the scale bar) and incorporate this information in the corresponding figure caption.**
*** Ensure all abbreviations are defined in the figure caption.**
*** The meaning of all error bars and how they were calculated should be described within the captions of all figures in which they occur."**

- Responses: The authors re-draw and change all figures to best comply with those issues.

**"Please do not make general references to the supplementary information. Please clearly specify which supplementary note, figure table etc the readers should consult."**
**"Please split the supplementary information into notes and refer to these individually and in numerical order in the main text of the manuscript (see supplementary information for more details). Please ensure that all notes are referred to in the manuscript and that all supplementary figures and tables etc are referred either in the main text of the article or the notes of the supplementary information."**

- Responses: The authors thoroughly revised the Supplementary Note along with figures and table therein. In the main text, all the Supplementary Figures, Table, and Notes are specifically mentioned in the right order.

**"We are committed to ensuring clarity and avoiding ambiguity in the mathematics in our papers. Consequently, please carefully check the mathematical terms throughout your manuscript (including labels on figures and figure captions) to ensure that it conforms strictly to the following guidelines. In mathematical terms, scalar variables (e.g. x, V, χ) and constants (e.g. π, ħ, e) should be typeset in italics, and vectors (such as r, the wavevector**

**k, or the magnetic field vector B) should be typeset in bold without italics. In contrast, subscripts and superscripts should only be italicized if they too are variables or constants. Those that are labels (such as the 'c' in the critical temperature, T_c, the 'F' in the Fermi energy, E_F, or the 'crit' in the critical current, I_crit) should be typeset in roman. Please also ensure the same convention is followed in figure labels, axes, and such. Additionally, to avoid doubt, unit dimensions should be expressed using negative integers (e.g. kg m^-1 s^-2 not kg/ms^2) or the word 'per'."**

- Responses: The authors revised all equations to perfectly comply witht the journal policy.

**"Please label each step using the a, b, c... convention and provide a brief description in the figure caption."**
**"Please define variables in the figure captions. Each caption should stand alone and not require reference to the main text to be understood. We have a 350 word limit for figure legends, therefore please provide more detail."**

- Responses: The Figure and corresponding text have been revised as the editor instructed.

**"* Please ensure all references are formatted in the Nature style.**
*** Please check the numbering of the references carefully. "**
**"For book publication please include location of the publisher."**

- Responses: All references are formatted in accordance with Nature style, and re-ordered as it is mentioned in the text. All book publications have the correct location of the publishers.

**"Please include the author contributions, competing interests, and data availability as separate statements."**

- Responses: The revised paper has separate statements for the (1) author contributions, (2) competing interests, and (3) data availability.
  In particular, all the raw training data used for this study has been made publicly available and shared on an endurable repository of the author, and the corresponding information has beed added in the Data Availability section as

  [Raw training data of nano tribocharging experiments adapted from the authors' prior work (18) are available at [https://sites.google.com/site/ichoddcse2017/home/Computational-Sci--Eng/nano-letters-2019]. All the computational programs are available upon proper request to the corresponding author.]

**"Please provide the supplementary information as a separate document.."**

- Responses: The authors papared and submitted the Supplementary Information as a separate document.

*** The Supplementary Information should be organised into the following subheaded sections, in this order:**
**- Supplementary Figures, labelled and referred to as Supplementary Figure 1, not Fig 1, throughout both the Supplementary Information and the main text**

**- Supplementary Tables, labelled and referred to as Supplementary Table 1, not Table 1, throughout both the Supplementary Information and the main text**
**- Supplementary Notes, numbered Supplementary Note 1, Supplementary Note 2, etc.**
**- Supplementary Discussion**
**- Supplementary Methods**
**- Supplementary References, which should be self-contained. That is, references mentioned in both the main text and the Supplementary Information should be part of both reference lists so that the Supplementary Information does not refer to the reference list in the main paper and vice versa. References cited in the Supplementary Information should be numbered sequentially from 1. They should be formatted in the same style as the main paper."**

- Responses: The revised Supplementary Information has the correct names of figures, table, and reference as instructed by the journal policy. They are accordingly mentioned throughout the main article and Supplementary Information.

**"*Please make sure that all supplementary notes are referred to (in order) in the main text of the article.**
***Please make sure that all supplementary figures, tables etc are referred to either in the main text of the article or the supplementary notes themselves."**

- Responses: The revised main article refers to the Supplementary Notes in order. Also, all the Supplementary Figures and Table are referred in order by main article and supplementary information.

**"Please call this supplementary note 1 and follow the same guidelines for all notes. Please also make sure to order your notes so that they can be cited in the order in the main article."**
**"Please label equations in the supplementary file as separate supplementary equations."**
**"Please call this supplementary note 2 and follow the same guidelines for all notes. Please also make sure to order your notes so that they can be cited in the order in the main article."**
**"Please call this supplementary note 3 and follow the same guidelines for all notes. Please also make sure to order your notes so that they can be cited in the order in the main article."**

- Responses: The authors re-named Supplementary Note as instructed by the Editor accordingly. The Notes are refered in order.

**"Please call supplementary figures as**
**"Supplementary Figure 1", Supplementary Figure 2", etc.. similarly for table and notes."**
**"Please make sure to update references to equations."**
**""Supplementary Table 1", Supplementary Table 2", etc.. similarly for figures and notes. Also cite in the main article and the SI accordingly"**

- Responses: In the main article and Supplementary Information, all figures and table are correctly referred according to the journal policy.