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MS #3165: Submission received for Makara Journal of Science

1 message

Editors of Makara Journal of Science <editors-science-3165@dcuischolarhub.bepress.com> Thu, Jul 24, 2025 at 10:41 PM
To: =?UTF-8?Q?=22Listiana_Satiawati_-_-=22?= <listianasatiawati@trisakti.ac.id>
Cc: The Authors <authors-science-3165@dcuischolarhub.bepress.com>, The Editors <editors-science-3165@dcuischolarhub.bepress.com>

A new submission for Makara Journal of Science has been uploaded by "Listiana Satiawati - -" <listianasatiawati@trisakti.ac.id>.

The authors are:
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The title is:
"Theory of Temperature-dependent Optical Conductivity of La0.7Ca0.3MnO3 Showing Metal to Insulator Transition"

The keywords are:
LCMO, MIT, optical conductivity, hopping parameters, magnetic correlations.
The disciplines are:
Condensed Matter Physics

The submission has been assigned #3165. Please refer to this number in any correspondence related to the submission.

Authors may check the status of the submission, submit revisions, and contact editors via the following link:

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Best regards,
The Editors
Makara Journal of Science

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Listiana satiawati <listianasatiawati@trisakti.ac.id>

3165 Revision of Proofreading

Makara Journal of Science <editor_mss@ui.ac.id> Mon, Apr 20, 2026 at 9:13 AM
To: Listiana satiawati <listianasatiawati@trisakti.ac.id>
Cc: "Dr. Ivandini Tribidasari A." <ivandini.tri@sci.ui.ac.id>

Dear Author,

Attached is the proofreading result of your manuscript entitled:

"Phenomenological Dynamical Mean-Field Theory of Temperature-Dependent Optical Conductivity and Metal Insulator Transition in La0.7Ca0.3MnO3
" (3165)

Please note the following points:
1. Please revise the manuscript in accordance with the proofreaders' comments.
2. Please align the reference list with the GFA guidelines (example attached).

Please submit the revised manuscript via the website no later than April 24, 2026.

Thank you for your cooperation.

Sincerely,

Puji Astuti
Editorial Assistant
Makara Science Journal

2 attachments

Format for Writing the Reference List.doc
43K

3165 Tracked Proofreading.docx
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Journal : Makara Journal of Science
Manuscript ID : MS# 3165
Title: Phenomenological Dynamical Mean-Field Theory of Temperature-Dependent Optical Conductivity and Metal Insulator Transition in $La_{0.7}Ca_{0.3}MnO_3$

There are some following issues that needs to be addressed:

Reviewer 5

Reviewer's Comments	**Author's Comments**
The current title inaccurately reflects the filename's incomplete formula and overlooks the methodological specifics. The authors may revise it to: "Phenomenological Dynamical Mean-Field Theory of Temperature-Dependent Optical Conductivity and Metal-Insulator Transition in $La_{0.7}Ca_{0.3}MnO_3$"	Many thanks to the reviewer for the suggestion regarding the title of our paper. Previously, we did not feel the need to explicitly mention the specific DMFT method in the title, as it would have made it too long. However, we can accept the title suggested by the reviewer as above. We have implemented this change in our revised manuscript.
The abstract lacks key quantitative results, such as the calculated Tc = 160 K versus experimental 260 K and discrepancies in the mid-energy regime. The authors should expand it by including these outcomes, fitted hopping coefficients (e.g., tb0 = 0.958 eV), and their implications for spectral weight transfer to ensure self-containment.	Thanks to the reviewer for the constructive comments and suggestions. We have implemented this suggestion in our revised manuscript while trying to keep the conciseness of the abstract. The revised abstract is the following: *Motivated to extend our previous theoretical study, we perform temperature-dependent optical conductivity calculation on $La_{0.7}Ca_{0.3}MnO_3$ in a wide photon energy range up to ~ 22 eV, to capture the metal to insulator transition, while still preserving in most way the correct temperature-dependent profile at higher photon energies. The system is modeled with a simple Mn–O coordination via the tight binding method with some hopping integrals being considered as functions of magnetization. Incorporating static Jahn-Teller effect, Coulomb-Hubbard and magnetic exchange interactions, apart from a quantitative difference in the calculated $T_c = 160$ K versus experimental 260 K and discrepancies in the mid-energy regime, ~~we are able to~~ our results reproduce the qualitative*

	trend of the temperature-dependent optical conductivity, especially for the low-and high-energy regimes, as observed in the experimental data. This qualitative agreement is achieved by setting the magnetization-dependent hopping parameters for the Mn–O hopping parameters, t_a *and* t_b*, to be* $t_{a(b)} = t_{a(b)}^{(0)} + t_{a(b)}^{(1)} M + t_{a(b)}^{(2)} M^2$*, with* $t_a^{(0)} = 0.958$ *eV,* $t_a^{(1)} = 0$*,* $t_a^{(2)} = 0.112$ *eV,* $t_b^{(0)} = 0.280$ *eV,* $t_b^{(1)} = 0$*, and* $t_a^{(2)} = 2.080$ *eV. Our results underline the importance of correlation effects due to interplay of lattice, charge, and magnetic degrees of freedom in determining the overall profile of temperature-dependent optical response of manganite, connecting the physics of high-energy optical response and the transport properties at the dc limit.*
Exclusion of La/Ca bands and t2g orbitals is asserted without quantitative validation against DFT or XPS data. The authors should add evidence, like projected DOS comparisons from literature or sensitivity analyses, to substantiate the Mn O model's sufficiency.	Our modelling aims to qualitatively capture the temperature-dependent trend of the optical conductivity of $La_{0.7}Ca_{0.3}MnO_3$ in a wide photon energy range up to ~ 22 eV, using only a minimum number of basis orbitals that are strongly-correlated such that they determine the temperature dependence of the optical conductivity of the system. For this reason, we only consider two e_g orbitals of the Mn ion and three p orbitals of the O ions in our model unit cell. Incorporating spins, overall, we have a set of 10 basis orbitals in our model. Of course, the neglect of the orbitals of the La/Ca atoms will result in our model being unable to reproduce the exact detailed profile of the optical conductivity in that very wide range of photon energy. But this is not our goal. To span the wide spectrum of energy while not incorporating all the atomic/Wannier orbitals of La/Ca atoms, we adjust the Mn-O hopping parameters in our model, accordingly. We argue that, in

	doing so, we take the effective Mn-O hopping parameters that have incorporated the effect of the presence of the orbitals of La/Ca atoms. To clarify this issue, we have added new sentences to our manuscript in the first paragraph of the Model and Method as follows: *We argue that these are the minimum number of basis orbitals that are strongly-correlated such that they determine the temperature dependence of the optical conductivity of the system.* Here, La band is ignored as it is considered not to contribute importantly to the electron dynamics in the energy region of our interest. *In order to span the wide spectrum of energy while not incorporating all the atomic or Wannier orbitals of La atoms, we then adjust the Mn-O hopping parameters in our model, accordingly. We argue that, in doing so, we take the effective Mn-O hopping parameters that have incorporated the effect of the presence of the orbitals of La atoms.*
The quadratic magnetization dependence in Eq. 5 remains phenomenological, lacking microscopic derivation. The authors should provide a theoretical basis (e.g., double-exchange perturbation) and sensitivity tests to affirm robustness beyond empirical fitting.	Relating the hopping parameters with magnetization is a phenomenological means of implementing the Anderson-Hasegawa's proposal stating that the electron hopping parameters between ions with magnetic moments depend on the relative orientations between the two magnetic moments. We have mentioned this in the introduction part of our previous manuscript and cited the relevant reference (Ref. [9]). In the **Anderson–Hasegawa double-exchange context**, the effective hopping amplitude between two sites depends on the angle between the local ionic spins θ. For two classical core spins $\mathbf{S}_i$ and $\mathbf{S}_j$, the electron hopping term is renormalized roughly as $t_{\text{eff}} \propto t_0 \cos\left(\frac{\theta}{2}\right)$ where t_0 is the bare hopping, and θ is the angle between the classical spins. This

	arises because the spinor overlap between neighboring sites depends on alignment. If the **magnetization** M is taken as a measure of average spin alignment (e.g., $M = \langle \cos(\theta) \rangle$ or a normalized ferromagnetic order parameter), then it's quite natural as a *phenomenological approximation* to express $t(M) \approx t_0 f(M)$, with $f(M)$ an increasing function of M. This reflects the physical intuition that *better alignment → easier hopping → larger effective kinetic bandwidth*. Assuming a polynomial dependence of $t(M)$ and truncating to leading terms is widely used in phenomenological modeling: $t(M) \approx t_0 + a\,M + b\,M^2 + \cdots$ Although for symmetry reasons (e.g., time-reversal invariance in collinear systems), often the **linear term may vanish,** and the first meaningful dependence is **quadratic in M**: $t(M) \approx t_0 + b\,M^2$, in our model, we keep the linear term $a\,M$, so that at the end, we can verify that the best fit, in fact, leads us to set the linear term to zero. This mirrors common Landau-Ginzburg type expansions, where expansion in terms of an order parameter M is truncated to the lowest nontrivial terms. Such expansions are not derived from first principles but capture *parametric trends* (enhanced hopping in ferromagnetic order) and are used in **phenomenological models of magnetoresistance, magneto-transport, and bandwidth control**.
The model's Tc = 160 K underestimates the experimental value without detailed quantification. The authors should include a subsection on parameter sensitivity (U, J_H, E_{JT}) and comparisons to multi-orbital DMFT for improved realism	Thank you for the question. The conclusion that our model's ferromagnetic Tc is ~160 K is based on our previous work (Ref [14]). We realize that, as far as getting the Tc right, our simple model seems inadequate. Some interaction terms may need to be added to improve Tc. We could play around with the model

	parameters (U, J_H, E_{JT}) to improve our model's Tc. However, doing so might mean sacrificing the general profile of the calculated optical conductivity, which we prefer not to do. Therefore, since getting the Tc right is not our goal, but rather we want to explore how the qualitative optical conductivity profile behaves with temperature changes in the ferromagnetic and paramagnetic regions, we argue that it is sufficient for us to compare our calculated results for T below and above our model's Tc (160 K), with experimental data for T below and above the experimental Tc (260 K).
Poor agreement in the 5.5-12 eV regime is acknowledged superficially. The authors should specify deficiencies (e.g., O-p dynamics) via partial DOS (Fig. 2) and propose extensions like dynamic Jahn-Teller phonons.	Thank you for your question. Below, we address the issue of discrepancies in the mid-energy region, and in general, to improve the resemblance of the detailed profile of our calculated optical conductivity as compared to the experimental data. We believe that, in order to capture all the detailed profiles of optical conductivity over a very wide photon energy range (0-22 eV), we must incorporate all atomic or Wannier orbitals of all atoms present in the LaMnO3 unit cell into our model. This can be done by first performing DFT calculations and then obtaining the tight-binding Hamiltonian parameters using a Wannierization package (such as Wannier90). This procedure will result in our tight-binding Hamiltonian matrix (i.e., the non-interacting part before adding the interaction terms) being very large, consisting of a much larger number of basis orbitals than the 10 in our current model. With this procedure, as far as the content of the non-interacting part of the Hamiltonian is concerned, we do not need to introduce any adjustable parameters, as they are all provided by the DFT+Wannierization calculation. On top of this complete non-interacting Hamiltonian, we then add the Hubbard

	and Hund interaction terms, using the parameters U and J_H, and solve the interacting problem within DMFT. While this procedure is ideal, it would require significantly more computational resources, which are currently beyond our capabilities. Therefore, we decided to perform a much simpler model that aims to capture only the general temperature-dependent trends, which reveal the important physics we want to emphasize, namely connecting the physics of high-energy optical response and the transport properties at the dc limit. Regarding dynamic Jahn-Teller phonons, we agree with the reviewer that dynamic Jahn-Teller phonons, when competing with the Anderson-Hasegawa double exchange mechanism, likely control what happens at the direct current (dc) limit, i.e., the metal-insulator transition. On the one hand, at high temperatures JT phonons are abundant, and magnetization is absent, delocalized electrons are scattered by JT phonons and can be trapped by forming localized polarons, leading to the system becoming an insulator. On the other hand, at low temperatures, the number of JT phonons is much lower, while magnetization tends to make the Mn-O electron hopping stronger, which in turn, makes the electrons more delocalized, resulting in a metallized phase. However, despite that rosy picture, a rigorous implementation of dynamical JT phonons and the Anderson-Hasegawa spin-dependent hopping parameters would result in a much more complex model, requiring much more sophisticated methods to solve it, and therefore, we choose not to do so at this time. To improve our manuscript regarding these issues, we have modified the relevant paragraph in the introduction

	as follows: ~~*A proper and rigorous treatment of the dynamic JT interaction in $La_{0,7}Ca_{0,3}MnO_3$ system is a challenging task, especially in addressing its role in the MIT phenomenon in this system.*~~ *We argue that the dynamic Jahn-Teller (JT) phonons, when competing with the Anderson-Hasegawa double exchange mechanism, lead to the occurrence of MIT. At high temperatures JT phonons are abundant, and magnetization is absent, itinerant electrons are scattered by JT phonons and can be trapped by forming localized polarons, leading to the system becoming an insulator. At low temperatures, the number of JT phonons is much lower, while magnetization tends to make the Mn-O electron hopping stronger, which in turn, makes the electrons more delocalized, resulting in a metallized phase. A rigorous modeling of such a competing mechanism would be a challenging task and require a more sophisticated method to solve it.* In this paper we shall not present such a treatment, rather, we propose that the as-yet-unknown detailed microscopic process of competition between the dynamic JT interaction and the DE driven FM correlation may be viewed phenomenologically as a process of renormalization of the Mn–O hopping parameters as magnetization develops in the system. In this way, the Mn–O hopping parameters become temperature dependent through the magnetization. ~~*We argue that in this system interaction of electrons with JT phonons trap the electrons to form polarons or quasi particles with low mobility, which in turn localize the electrons to some degree, making the system behave as insulator or insulator-like over a wide range of temperature.*~~ *Going from high to low temperature FM correlation starts to develop. This stimulates larger hopping probability via*

	DE mechanism. Hopping of Mn electrons via oxygen by DE mechanism is large if electron spins are aligned as postulated by Anderson and Hasegawa [9]. Hopping integral is roughly inversely proportional to temperature.
DOS analysis (Figs. 2-3) insufficiently integrates velocity matrix contributions from Eq. 4. The authors should decompose σ(ω) quantitatively across regimes, with convergence tests to valid	Our DOS analysis in Figure 2-3 serves only as a rough guide to indicate the possible electronic transitions corresponding to optical conductivity peaks without regard to spectral weights. Thus, when discussing DOS in relation to optical conductivity, we have not yet addressed the role of velocity matrices in controlling the spectral weights of optical conductivity. The actual spectral weights of optical conductivity peaks must, of course, be derived from careful calculations applying Equation 4 where velocity matrices are involved, which we discuss elsewhere.

Journal : Makara Journal of Science
Manuscript ID : MS# 3165
Title: Phenomenological Dynamical Mean-Field Theory of Temperature-Dependent Optical Conductivity and Metal Insulator Transition in $La_{0.7}Ca_{0.3}MnO_3$

There are some following issues that needs to be addressed:

Reviewer 7

Reviewer's Comments	Author's Comments
If this manuscript is planned to be published right after this report, it is suggested that authors provide short description of what they actually do in ref 14. The study in reference no. 14 is about manganite compound which has been extensively studied before. In this study it is expanded with the influence of temperature and doping function in the extended photon energy range from 0 to 22 eV. This manuscript proposes a model and calculation in the form of a Hamiltonian in dynamic mean field theory to explain the phenomenon of the emergence of spectral weight transfer in the $La_{1-x}Ca_xMnO_3$ system which transforms from a paramagnetic insulator to a ferromagnetic metal in a wide energy regime referring to the experimental study in reference 13. It is proven that the important role of the oxygen element in mediating electron jumps between Manganese elements to determine the optical conductivity structure. The mathematical model was constructed using a Hamiltonian composed of kinetic parts, consisting of 10 orbitals from the $La_{1-x}Ca_xMnO_3$ crystal structure, related to Jahn Teller spitting, the Coulomb repulsions between the upper and lower Mn_{eg} orbitals, and double-exchange magnetic interactions. This resulted in a model to explain the structure and spectral weight transfer that occurs in the optical	Thank you very much for the reviewer's positive response. Yes, our current manuscript presents an extended work of our previous work published in Ref. 14. The work in Ref. 14 itself is intended to theoretically explain the temperature-dependent optical conductivity profile of $La_{1-x}Ca_xMnO_3$ for x = 0.3, highlighting the spectral weight transfer between low, medium, and high photon energy regions in the range 0–22 eV as shown by the experimental data from Ref. 13. The proposed model in Ref. 14 is essentially the same as that used in the current manuscript, where the non-interacting or the kinetic part of the Hamiltonian is constructed within a tight-binding model using 10 basis orbitals taken from 2 Mn-d e_g and 3 O-2p orbitals incorporating spin degrees of freedom. On top of the non-interacting part, we added the on-site Coulomb-Hubbard repulsion terms for the two Mn-d e_g orbitals and the Hund's coupling between the Mn ion spins (from the t_{2g} electrons in the Mn ion) and the spins of the itinerant electrons. The model was then solved within the Dynamical Mean-Field Approximation/Theory. The main difference between our previous work published in Ref. 14 and our current work lies in the expressions of the phenomenological magnetization-dependent Mn-O hopping parameters (t_a and t_b). In the previous work, we

conductivity of $La_{1-x}Ca_xMnO_3$ for x = 0.3, with the inclusion of the O_{2p} orbital in the model.	assumed that t_a and t_b depend linearly on the magnetization (M). It turned out that, while the model was able to correctly explain the spectral weight transfers between the low, middle, and high photon energy regions, it failed to capture the metal-insulator transition at the direct current (dc) limit. In our current work, we propose that t_a and t_b depend quadratically on the magnetization (M). In addition, we reconsider the detailed expression of the non-perturbed part of the Hamiltonian. With this improved and more justified phenomenological assumptions, our current model can explain the spectral weight transfer between the low and high photon energy regions correctly and qualitatively capture the metal-insulator transition in the dc limit.

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3165 Revision of Proofreading

Listiana satiawati <listianasatiawati@trisakti.ac.id> Thu, Apr 23, 2026 at 11:30 AM
To: Makara Journal of Science <editor_mss@ui.ac.id>

Dear Editor MJS,
We have sent the revised grammar and reference writing as recommended.
Thankyou.
Listiana Satiawati
[Quoted text hidden]

UNIVERSITAS TRISAKTI

Listiana satiawati <listianasatiawati@trisakti.ac.id>

#3165 Publication Fee Invoice - Makara Journal of Science

2 messages

Makara Journal of Science <editor_mss@ui.ac.id> Wed, Apr 1, 2026 at 2:55 PM
To: listianasatiawati@trisakti.ac.id
Cc: "Dr. Ivandini Tribidasari A." <ivandini.tri@sci.ui.ac.id>

Dear Author,

We are pleased to inform you that your manuscript entitled "**Phenomenological Dynamical Mean-Field Theory of Temperature-Dependent Optical Conductivity and Metal Insulator Transition in La0.7Ca0.3MnO3**" (3165) has been accepted for publication in the Makara Journal of Science.

In accordance with the journal's publication policy, an Article Processing Charge (APC) is required to proceed with the production and publication of your article.

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Payment Deadline: April 15, 2026

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We sincerely appreciate your contribution to Makara Journal of Science and look forward to sharing your research with our readership worldwide.

Thank you for the cooperation.

Sincerely yours,

Chief Editor
Makara Journal of Science
Prof. Dr. Ivandini Tribidasari A.

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Dear Ms. Listiana Satiawati
Petroleum Engineering Department, Faculty of Earth and Energy Technology, Universitas Trisakti
Email: listianasatiawati@trisakti.ac.id

We would like to thank you for your trust to submit your article to be published in Makara Journal of Science. According to the procedures of publishing articles in scientific journals, we sent your article to reviewers to assess its feasibility prior to publication in our journal.

We are happy to inform you that your article, titled "**Phenomenological Dynamical Mean-Field Theory of Temperature-Dependent Optical Conductivity and Metal-Insulator Transition in La0.7Ca0.3MnO3**" (3165) is accepted for publication in Makara Journal of Science on volume 30, number 2, June 2026 edition.

Kindly visit our website at https://scholarhub.ui.ac.id/science/ to access our published articles.

Thank you for the cooperation.

April 30, 2026

Best Regards,

Prof. Dr. Ivandini Tribidasari Anggraningrum,
Chief Editor Makara Journal of Science