Paper Submission Form - SAIP2025 Proceedings

Sections A, C, D, and E must be completed by all authors (including students) who submit papers. Section B is compulsory for students who submit manuscript(s).

Section A: Paper Submission Information

Paper/Abstract ID	420
Paper title	Densiity functional theory study on the effect of pressure on structural, mechanical and phonon properties of A15 Mn3Ru alloy
Corresponding Author Name & Surname:	Mr Bhila Oliver Mnisi
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Section B: For Students & Supervisors

Supervisor Name & Surname:	Dr Malebo Mariam Tibane
Supervisor Email Address:	tibanmm@unisa.ac.za

For this paper, the supervisor must agree/disagree with the following statements.

	Yes	No
1. I am aware that the above-mentioned paper is being submitted for possible publication in the Proceedings of the SAIP Conference. I am satisfied that the presented work is that of the listed authors. I hereby give consent to the submission		
2. I have proof-read the manuscript		
3. I am satisfied that the manuscript is written in appropriate English and is sufficiently free of grammatical and spelling errors		
4. I am familiar with the required manuscript format ("House Style"), and I am satisfied that this manuscript meets the criteria. I am aware that manuscripts not conforming with House Style may be desk rejected		
5. I am satisfied that the scientific content of this manuscript is of sufficient standard for it to be considered for publication in the Proceedings of the South African Institute of Physics Conference Proceedings		

Student Name & Surname: …Mr Bhila Oliver Mnisi   Signature: ………………………..……   Date: 30-07-2025 ….……..

Supervisor Name & Surname: Dr Malebo Meriam Tibane   Signature: ……………………..………..   Date: 31-07-2025 ….…….…

Section C: Suggested Reviewers

Obtaining the two referee reports necessary for DHET subsidy is an onerous task.

Please provide the names and contact details of three qualified South African and/or international referees. Referees should have a PhD and expertise in the relevant area of Physics. Do not recommend referees who have co-authored a work with any of the authors on the manuscript within the past five (5) years. Manuscripts without three recommended referees may be subject to desk rejection.

Suggested Reviewers in your Research Field (Both local & international)		
	Reviewer Names & Surname	**Reviewer's Email Address(es)**
Suggested reviewer #1	Prof Nithaya Chetty	nithaya.chetty@wits.ac.za
Suggested reviewer #2	Prof Lesley Cornish	Lesley.Cornish@wits.ac.za
Suggested reviewer #3	Dr Refilwe Mapasha	edwin.mapasha@up.ac.za

Section D: Declaration of Novelty and Use of AI

__The authors declare that this article is original, and AI tools (such as ChatGPT) were used occasionally for paraphrasing and correcting grammatical errors

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How is this submitted manuscript scientifically novel?

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_This manuscript provides insights in finding novel materials for high-temperature structural application using density functional theory technique. This manuscript specifically investigates the novel A15 Mn_3Ru under high pressure for the first time. It was observed that Mn_3Ru has a negative heat of formation indicating thermodynamic stability at zero pressure. This leads to feasible experimental synthesis at zero pressure. We find that the Mn_3Ru alloy is mechanically stable from 100 GPa to 200 GPa. On the other From the phonon spectra, we note the absence of imaginary modes, indicating dynamical stability. Furthermore, at higher pressures, the melting point temperature of this alloy increases. Overall, pressure significantly enhances the mechanical and dynamic properties of Mn_3Ru, supporting its use in high-temperature structural applications especially in hot-section component of a gas turbine engine.

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Please see the Author Guidelines for the AI use policy.

How was AI used in the generation of this manuscript?

___The AI tool such as ChatGPT was used occasionally for paraphrasing and correcting grammatical errors.

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Section E: Plagiarism

	Yes
I am aware that plagiarism detection software may be used on my manuscript.	X