

# 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                    |                                                                                                                                                         |
| Paper title                          | First-principles study of the Structural, Mechanical, Dynamical, Electronic and Lattice Thermal Conductivity properties of HfSnPt: A half-Heusler alloy |
| Corresponding Author Name & Surname: | Ibrahim Omer Abdallah Ali                                                                                                                               |
| Corresponding Author Email Address:  | ibraphysics@gmail.com                                                                                                                                   |

## Section B: For Students & Supervisors

|                            |                     |
|----------------------------|---------------------|
| Supervisor Name & Surname: | M M 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: ...Ibrahim Ali.....  
Date: 31-07-2025

Signature:

31-7-2025

Supervisor Name & Surname: ...M M Tibane.....

Signature: .....

31-07-2025

Date: .....

## Suggested Reviewers in your Research Field (Both local & international)

|  | Reviewer Names & Surname | Reviewer's Email Address(es) |
|--|--------------------------|------------------------------|
|--|--------------------------|------------------------------|

|                       |                 |                           |
|-----------------------|-----------------|---------------------------|
| Suggested reviewer #1 | Refilwe Mapasha | edwin.mapasha@up.ac.za    |
| Suggested reviewer #2 | Dongho Moise    | donghomoise@gmail.com     |
| Suggested reviewer #3 | Mahlaga Molepo  | mahlaga.molepo@wits.ac.za |

## 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.**

## Section D: Declaration of Novelty and Use of AI

**How is this submitted manuscript scientifically novel?**

This submitted manuscript is scientifically novel as it presents a comprehensive first-principles investigation of the Half-Heusler (HH) compound HfSnPt, a non-toxic alloy with potential for high-temperature applications. While previous studies have examined related compounds such as HfPtSn and confirmed their thermodynamic stability and semiconducting behavior, the detailed mechanical, vibrational, and thermal transport properties of HfSnPt remain largely unexplored. This work addresses that gap by systematically evaluating the phase stability, elastic constants, electronic structure, phonon dispersion, and lattice thermal conductivity of HfSnPt using density functional theory (DFT) calculations via the VASP software. The results provide new insights into the fundamental physical properties of HfSnPt, contributing valuable data to the field of thermoelectric and high-temperature materials research.

**Please see the Author Guidelines for the AI use policy.**

**How was AI used in the generation of this manuscript?**

Artificial intelligence tools, specifically ChatGPT by OpenAI, were used solely to assist with language editing, paraphrasing, grammar correction, and formatting. These tools were not involved in the scientific design, data generation, analysis, or interpretation. The authors have thoroughly reviewed and verified the final content to ensure its accuracy, integrity, and originality.

Section E: Plagiarism

|                                                                             |     |
|-----------------------------------------------------------------------------|-----|
|                                                                             | Yes |
| I am aware that plagiarism detection software may be used on my manuscript. | ✓   |