

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	528
Paper title	Assessing the Freysoldt, Neugebauer & van de Walle (FNV) and Kumagai–Oba (KO) finite-size corrections for Ce-vacancy complexes in diamond
Corresponding Author Name & Surname:	Dr Wynand Dednam
Corresponding Author Email Address:	dednaw@unisa.ac.za

Section B: For Students & Supervisors

Supervisor Name & Surname:	
Supervisor Email Address:	

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: Signature: Date:

Supervisor Name & Surname: Signature: Date:

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	Dr Refilwe Mapasha	edwin.mapasha@up.ac.za
Suggested reviewer #2	Dr Mahlaga Molepo	mahlaga.molepo@wits.ac.za
Suggested reviewer #3	Dr Walter Meyer	wmeyer@up.ac.za

Section D: Declaration of Novelty and Use of AI

How is this submitted manuscript scientifically novel?

The manuscript compares two techniques for correcting finite-size effects in charged defect DFT calculations on Lanthanide doped diamond. To our knowledge no such comparative calculations have been performed on Lanthanide-doped diamond. This comparison allows for a quick diagnostic of whether a defect is deep or shallow using just the electrostatic potential extracted from the converged DFT calculation. Recent works (see refs. 21 and 23 of the attached manuscript) have employed the FNV correction without providing details of the correction results in either their main manuscript or the supplementary material.

Please see the Author Guidelines for the AI use policy.

How was AI used in the generation of this manuscript?

AI was used to debug the python code interfacing the SPINNEY API needed to post-process the CASTEP binary output files. It was also used to improve the readability of a few of the longer sentences in the manuscript.

Section E: Plagiarism

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