This declaration concerns the article entitled:

Candidate photoferroic absorber materials for thin-film solar cells from naturally occurring minerals: enargite, stephanite, and bournonite

Pages 107-118 of thesis

Publication status (tick one)									
draft manuscript		**Submitted**		**In review**		**Accepted**		**Published**	X

Publication details (reference)	Wallace, S., Svane, K., Huhn, W., Zhu, T., Mitzi, D., Blum, V. and Walsh, A. (2017). Candidate photoferroic absorber materials for thin-film solar cells from naturally occurring minerals: enargite, stephanite, and bournonite. *Sustainable Energy & Fuels*, 1(6), pp.1339-1350.
Candidate's contribution to the paper (detailed, and also given as a percentage).	*Formulation of ideas (50%):* The original idea for the criteria used in this study to screen minerals for candidate photoactive ferroelectrics for photovoltaic (PV) applications (dark streak colour and polar space group) was provided by A. Walsh. The dataset of minerals was also provided by A. Walsh. Ideas for further investigations into the properties of the candidates for PV applications were from myself (S. Wallace) with support when performing the electronic structure calculations with FHI-aims provided by V. Blum, W. P Huhn and T. Zhu. *Design of methodology (50%):* As this study involved a small dataset (<200 minerals) novel screening techniques were not required. After identifying the candidate materials subsequent electronic structure calculations were primarily conducted during a collaboration visit to Duke University with developers of the FHI-aims electronic structure software package. Spin-orbit coupling was incorporated into routines used in this study to calculate the optical dielectric constant by T. Zhu. Before applying this methodology, S. Wallace assisted in testing and benchmarking the modified routines. Otherwise, existing routines in the FHI-aims software package were utilised in this study. *Experimental work (75%):* The screening process was conducted by S. Wallace. Most calculations in the work were performed by S. Wallace, the only exceptions being those of electron localisation functions (presented in the supplemental material) and spontaneous lattice polarisations (presented in the main body of the paper and the supplemental material) which were performed by K. Svane at the University of Bath using the VASP electronic structure software package. The Python script used to obtain fits to the band extrema to compute charge carrier effective masses with band structures in the format outputted by FHI-aims was written by T. Zhu and used with permission. *Presentation of data in journal format (75%):* The first draft of the manuscript was written by S. Wallace. Discussions were provided by all co-authors throughout the study and all helped with proof-reading and preparing the manuscript for submission.
Statement from Candidate	This paper reports on original research I conducted during the period of my Higher Degree by Research candidature.

Signed	S. Wallace	**Date**	01.11.18