


This declaration concerns the article entitled:									
Candidate photoferroic absorber materials for thin-film solar cells from naturally occurring minerals: enargite, stephanite, and bournonite									
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Candidate's contribution to the paper (detailed, and also given as a percentage).	<p>The original idea for the criteria used in this study to screen minerals for photovoltaic (PV) applications (dark streak colour and polar space group) was provided by A. Walsh. The screening procedure was then conducted by S. Wallace and ideas for further investigations into the properties of the candidates for PV applications were from S. Wallace. 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: V. Blum, W. P Huhn and T. Zhu.</p> <p>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. Support when performing the electronic structure calculations with FHI-aims was provided by V. Blum, W. P Huhn and T. Zhu and discussions were provided by all co-authors throughout this study.</p>								
Statement from Candidate	This paper reports on original research I conducted during the period of my Higher Degree by Research candidature.								
Signed						Date	01.11.18		