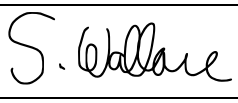
Appendix B: Statement of Authorship

<table>
<tr><th colspan="10">This declaration concerns the article entitled:</th></tr>
<tr><td colspan="10">Finding a junction partner for candidate solar cell absorbers enargite and bournonite from electronic band and lattice matching

Pages 123 - 131 of thesis</td></tr>
<tr><td colspan="10">Publication status (tick one)</td></tr>
<tr><td>draft manuscript</td><td>X</td><td>Submitted</td><td></td><td>In review</td><td></td><td>Accepted</td><td></td><td>Published</td><td></td></tr>
<tr><td>Publication details (reference)</td><td colspan="9">Finding a junction partner for candidate solar cell absorbers enargite and bournonite from electronic band and lattice matching
SK Wallace, KT Butler, Y Hinuma, A Walsh</td></tr>
<tr><td>Candidate's contribution to the paper (detailed, and also given as a percentage).</td><td colspan="9">Formulation of ideas (70%): The dataset of candidate junction partners was collated by K. Butler and the ElectronLatticeMatch python libraries were also developed by K. T. Butler. The idea to use this existing tool to look for junction partners with specific band offsets (cliff- or spike-like) for the absorber materials identified in chapter 5 of this thesis was from myself (S. Wallace) where the screening criteria used in the study was chosen by S. Wallace and informed by previous works in the literature on other absorber materials (CdTe, ZnSnN2 and CIGS).

Design of methodology (50%): As mentioned in the previous section, this work made use of a python library developed by K. Butler (ElectronLatticeMatch). This was incorporated into an interactive workflow by S. Wallace to screen for candidate junction partners in this study with screening criteria chosen by S. Wallace. Non-polar, symmetric slab models used for the calculations of ionisation potential in this study were cut by Y. Hinuma using methodology developed by Y. Hinuma. Ionisation potentials of the slab models were calculated using existing MacroDensity python libraries.

Experimental work (70%):
For this study, S. Wallace performed electronic structure calculations with the VASP software package for the volume relaxation of bulk unit cells from which Y. Hinuma generated slab models. S. Wallace also performed electronic structure calculations for the slab models and processed outputs from the electronic structure calculations with the MacroDensity and ElectronLatticeMatch python libraries. Throughout this work, support and discussions were provided by K. T. Butler for utilising the python libraries and performing electronic structure calculations for the slab models.

Presentation of data in journal format (70%): The first draft of the manuscript was prepared by S. Wallace and all co-authors provided support when finalising the manuscript for submission.</td></tr>
<tr><td>Statement from Candidate</td><td colspan="9">This paper reports on original research I conducted during the period of my Higher Degree by Research candidature.</td></tr>
<tr><td>Signed</td><td colspan="5">  </td><td>Date</td><td colspan="3">15/11/18</td></tr>
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