**Investigating the Structure-Function Relationship in Triple Cation Perovskite Nanocrystals for Light-Emitting Diode Applications**

Parth Vashishtha†\*, Sjoerd A. Veldhuis‡, Sai S. H. Dintakurti†∥¦, Nicole L. Kelly∥, Benjamin E. Griffith∥, Alasdair A. M. Brown‡§, Mohammed Suhail Ansari†, Annalisa Bruno‡, Nripan Mathews†‡, Yanan Fang†, Tim White†, Subodh G. Mhaisalkar†‡\*, John V. Hanna∥†\*

†School of Materials Science and Engineering, Nanyang Technological University (NTU), 50 Nanyang Avenue, Singapore 639798, Singapore.

‡Energy Research Institute @NTU (ERI@N), Research Techno Plaza, X-Frontier Block, Level 5, 50 Nanyang Drive, Singapore 637553, Singapore.

∥Department of Physics, University of Warwick, Coventry CV4 7AL, UK.

¦Interdisciplinary Graduate School, Nanyang Technological University (NTU), 50 Nanyang Avenue, Singapore 639798, Singapore.

§School of Engineering, Faculty of Engineering and Physical Sciences, University of Southampton, Southampton SO17 1BJ, UK.

This document serves as instructions for the location of the data within the directory **Hanna\_TripleCation\_Repository\_Data** available from the University of Warwick open access research data repository, WRAP (Warwick Research Archive Portal). This data directory contains the raw data files for all data presented in the manuscript entitled “Investigating the Structure-Function Relationship in Triple Cation Perovskite Nanocrystals for Light-Emitting Diode Applications“

The directory is separated into the subdirectories below:

**LED EQE Data**

This contains the Origin and Excel ASCII data of the LED EQE Data for **CsX** where **X** is the amount of Cs doping.

**LED Stability**

This folder contains the Origin ASCII data for the LED stability data and the raw text files for **CsX** where **X** is the amount of Cs doping.

**NMR**

This contains 8 subfolders, the folder names are **XX\_Date\_YY**, where **XX** is the nucleus, **Date** is the date the data was collected in the format YYMMDD and **YY** is the sample, field or experiments contained within the folder. Bruker TOPSPIN software is required to process the data files, with the exception of the data contained in 133Cs\_Infinity which requires ssNake or Varian-Chemagnetics SPINSIGHT to process the data.

**Optical Properties**

This folder contains the sample photo, the **UV-PL Triple Cation** Origin file and three subfolders **PL**, **TRPL** and **UV-Vis**. The **PL** folder contains the photoluminescence data for **CsX** where **X** is the amount of Cs doping, and the photoluminescence Origin file. **TRPL** contains the short range data for all Cs doping levels. **UV-Vis** contains the raw files for the UV-Vis data for **CsX** where **X** is the amount of Cs doping.

**TEM**

The folder contains the TIFF files for **X Cesium**, where **X** is the amount of Cs doping.

**XRD**

This contains the ASCII data in Origin files for the **Pure CsPbBr3** and **XRD** data and the .xy files for **CsX** and **CsPbBr3**, where **X** is the Cs doping.

All text documents and the .xy XRD data can be opened using Excel, OriginPro or any text editor. OPJU files can be opened in Origin or OriginPro.