



*Citation for published version:*

Davies, D, Savory, C, Frost, JM, Scanlon, DO, Morgan, B & Walsh, A 2020, 'Descriptors for Electron and Hole Charge Carriers in Metal Oxides', *Journal of Physical Chemistry Letters*, vol. 11, no. 2, pp. 438-444.  
<https://doi.org/10.26434/chemrxiv.11214914.v1>, <https://doi.org/10.1021/acs.jpcllett.9b03398>

*DOI:*

[10.26434/chemrxiv.11214914.v1](https://doi.org/10.26434/chemrxiv.11214914.v1)  
[10.1021/acs.jpcllett.9b03398](https://doi.org/10.1021/acs.jpcllett.9b03398)

*Publication date:*

2020

*Document Version*

Peer reviewed version

[Link to publication](#)

This document is the Accepted Manuscript version of a Published Work that appeared in final form in The Journal of Physical Chemistry Letters, copyright © American Chemical Society after peer review and technical editing by the publisher. To access the final edited and published work see <https://doi.org/10.1021/acs.jpcllett.9b03398>

**University of Bath**

## **Alternative formats**

If you require this document in an alternative format, please contact:  
[openaccess@bath.ac.uk](mailto:openaccess@bath.ac.uk)

### **General rights**

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

### **Take down policy**

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

# Descriptors for Electron and Hole Charge Carriers in Metal Oxides

Daniel W. Davies,<sup>\*,†,||</sup> Christopher N. Savory,<sup>‡,||</sup> Jarvist M. Frost,<sup>¶</sup> David O. Scanlon,<sup>‡,||</sup> Benjamin J. Morgan,<sup>§,||</sup> and Aron Walsh<sup>\*,†,||</sup>

<sup>†</sup>*Department of Materials, Imperial College London, London SW7 2AZ, United Kingdom*

<sup>‡</sup>*Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, United Kingdom*

<sup>¶</sup>*Department of Physics, Imperial College London, London SW7 2AZ, UK*

<sup>§</sup>*Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom*

<sup>||</sup>*The Faraday Institution, Quad One, Harwell Science and Innovation Campus, Didcot, UK*

<sup>⊥</sup>*Diamond Light Source Ltd., Diamond House, Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, United Kingdom*

<sup>#</sup>*Department of Materials Science and Engineering, Yonsei University, Seoul 03722, Korea*

E-mail: d.davies16@imperial.ac.uk; a.walsh@imperial.ac.uk

## Supplementary Information

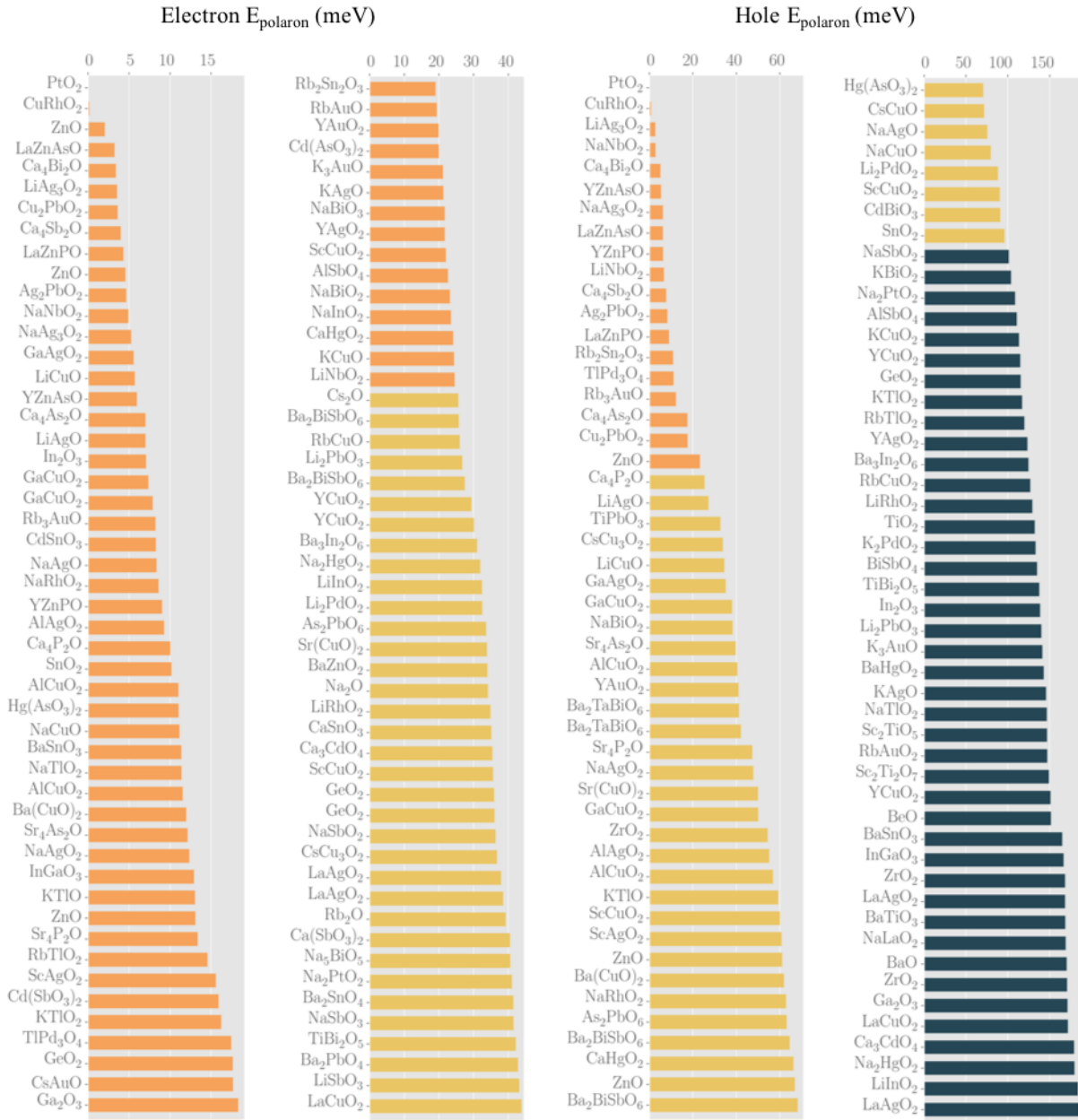


Figure S1: Electron and hole polaron binding energies calculated using the effective masses and dielectric constants from public data-sets. Some compositions have multiple entries due to polymorphism.

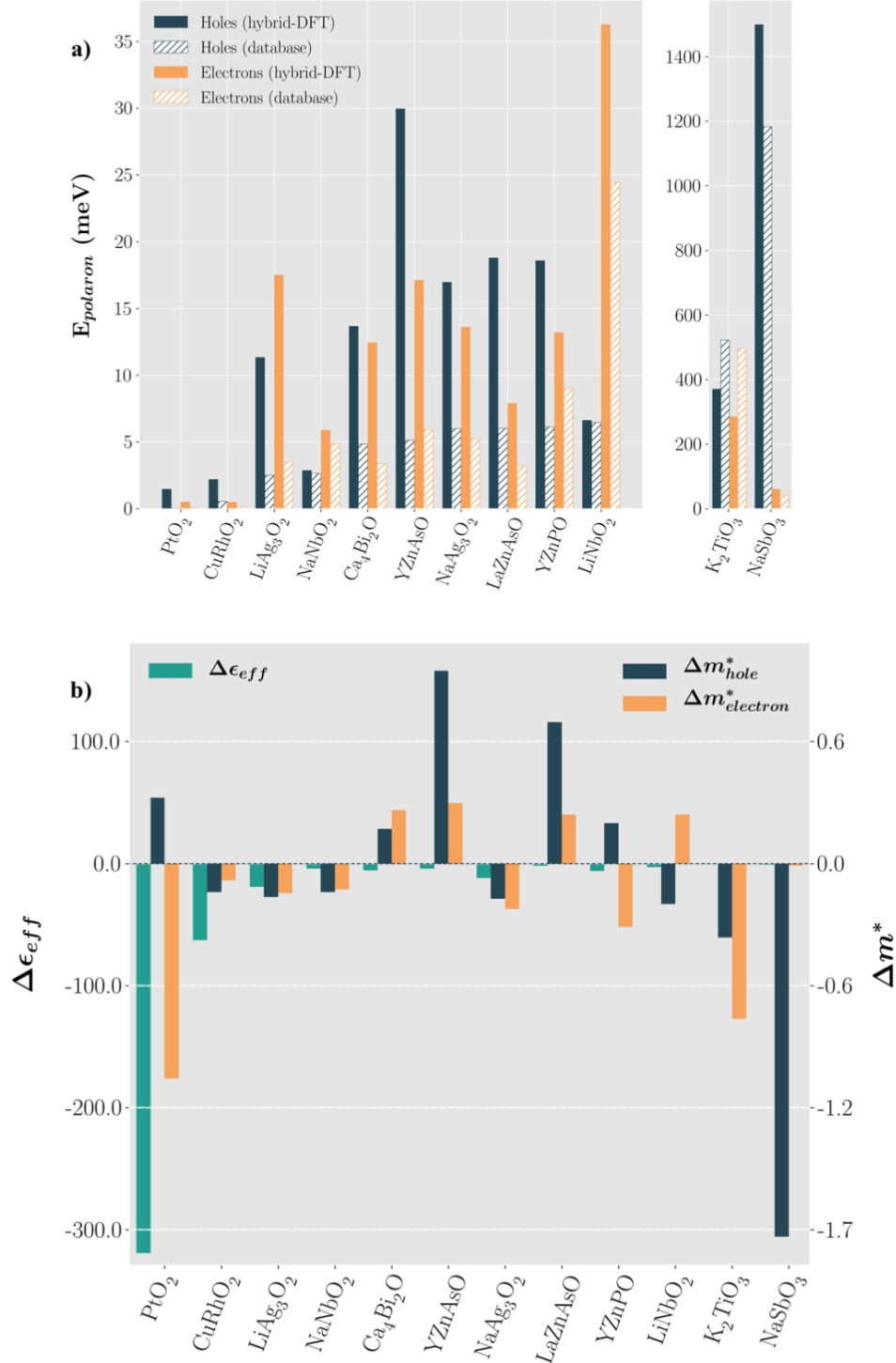


Figure S2: a) Polaron energy ( $E_{polaron}$ ) values as calculated using hybrid-DFT (solid bars) and database (hatched bars) for electrons (orange bars) and holes (blue bars). b) Absolute difference (database derived minus Hybrid-DFT derived) in  $\epsilon_{eff}$  (green bars) and effective mass ( $m^*$ ) for electrons (orange bars) and holes (blue bars).

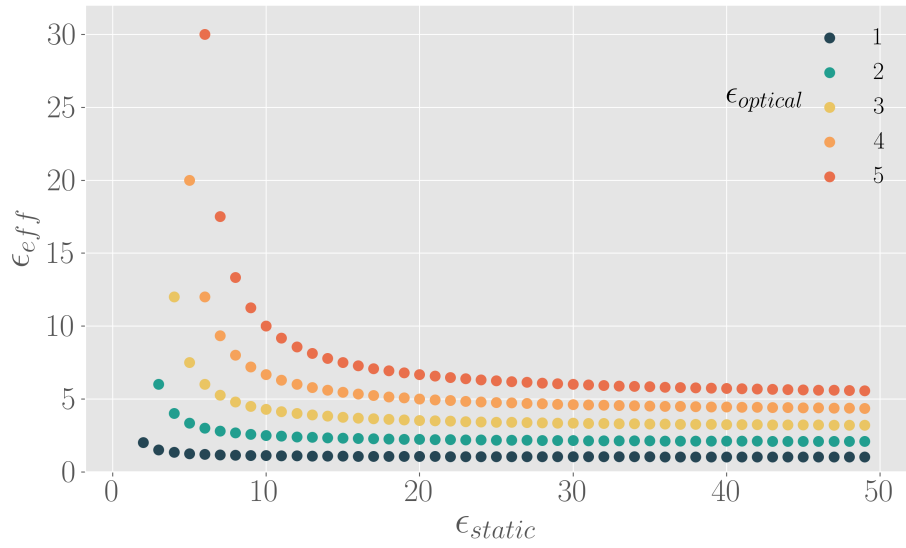


Figure S3: Visualization of the variation of  $\epsilon_{eff}$  (y-axis) with  $\epsilon_s$  (x-axis) at different fixed values of  $\epsilon_\infty$ . For  $\epsilon_s > 20$  the system is in a strong screening regime where  $\epsilon_{eff}$  shows little variation.