Descriptors for Electron and Hole Charge Carriers in Metal Oxides

Daniel W. Davies,[*,†,‖] Christopher N. Savory,[‡,‖] Jarvist M. Frost,[¶] David O. Scanlon,[‡,‖] Benjamin J. Morgan,[§,‖] and Aron Walsh[*,†,‖]

†*Department of Materials, Imperial College London, London SW7 2AZ, United Kingdom*

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

¶*Department of Physics, Imperial College London, London SW7 2AZ, UK*

§*Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom*

‖*The Faraday Institution, Quad One, Harwell Science and Innovation Campus, Didcot, UK*

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

#*Department of Materials Science and Engineering, Yonsei University, Seoul 03722, Korea*

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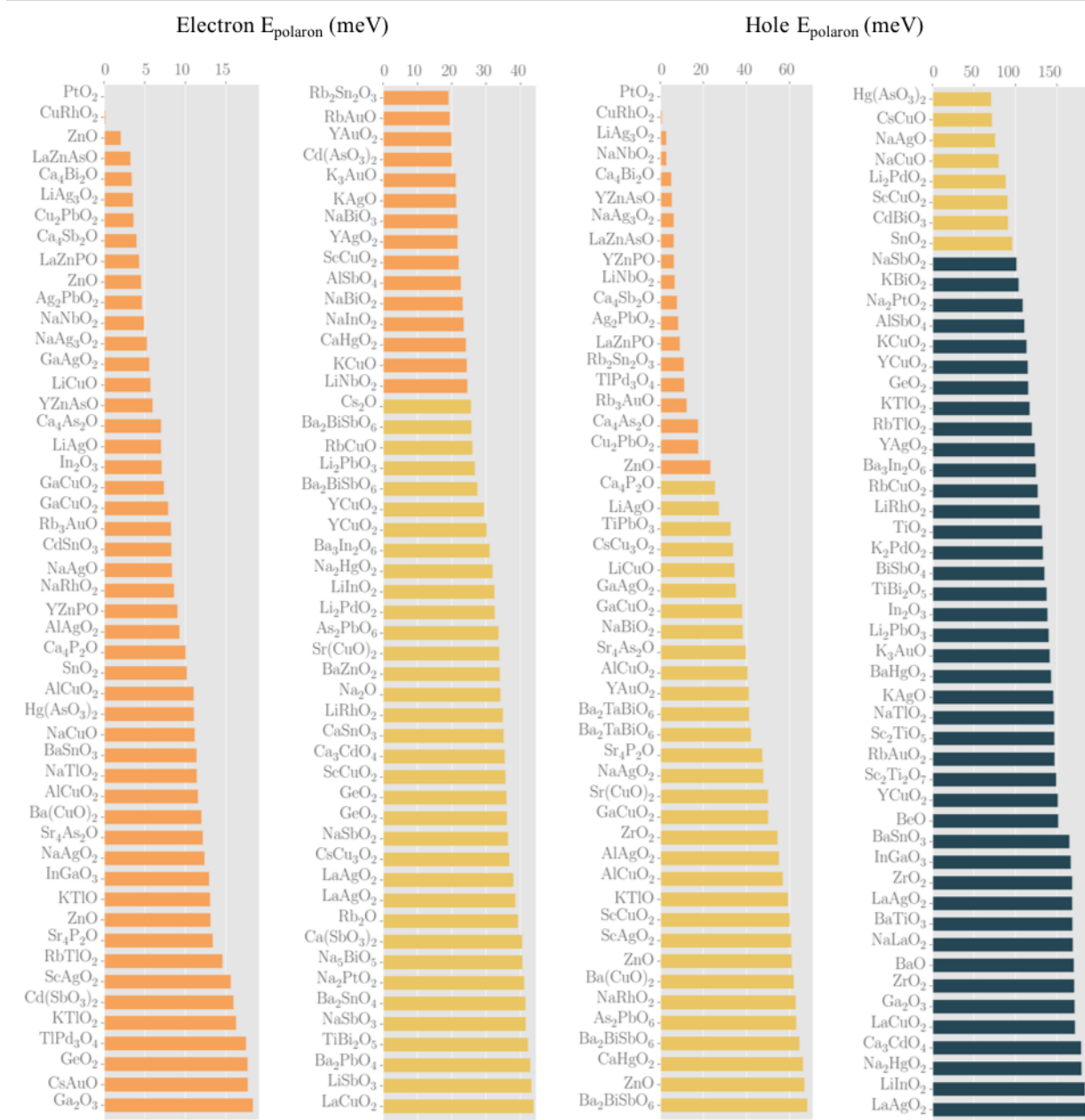
Supplementary Information

1

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.
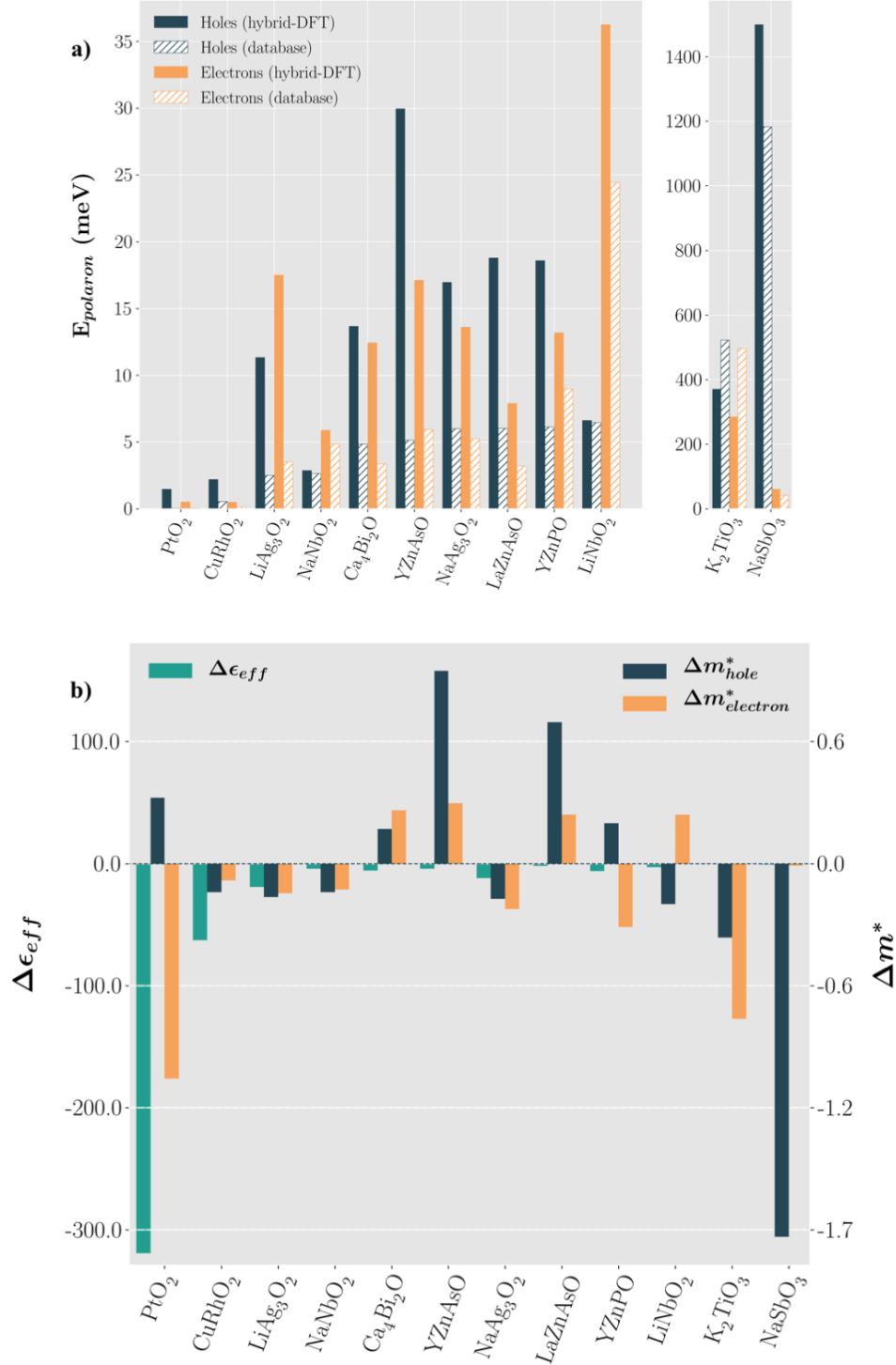
Figure S2: a) Polaron energy ($E_{polaron}$) values as calculated using hybrid-DFT (solid bars) and database (hatched bars) for electrons (orange bars) and holes (blue bars). b) Absolute difference (database derived minus Hybrid-DFT derived) in ϵ_{eff} (green bars) and effective mass (m^*) for electrons (orange bars) and holes (blue bars).
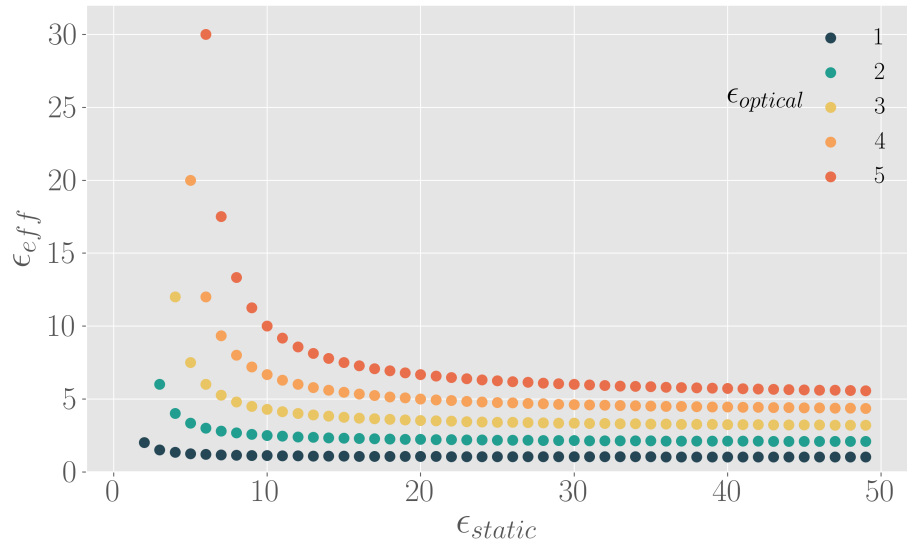
Figure S3: Visualization of the variation of ϵ_{eff} (y-axis) with ϵ_s (x-axis) at different fixed values of ϵ_∞. For $\epsilon_s > 20$ the system is in a strong screening regime where ϵ_{eff} shows little variation.