Descriptors for Electron and Hole Charge Carriers in Metal Oxides

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Supplementary Information

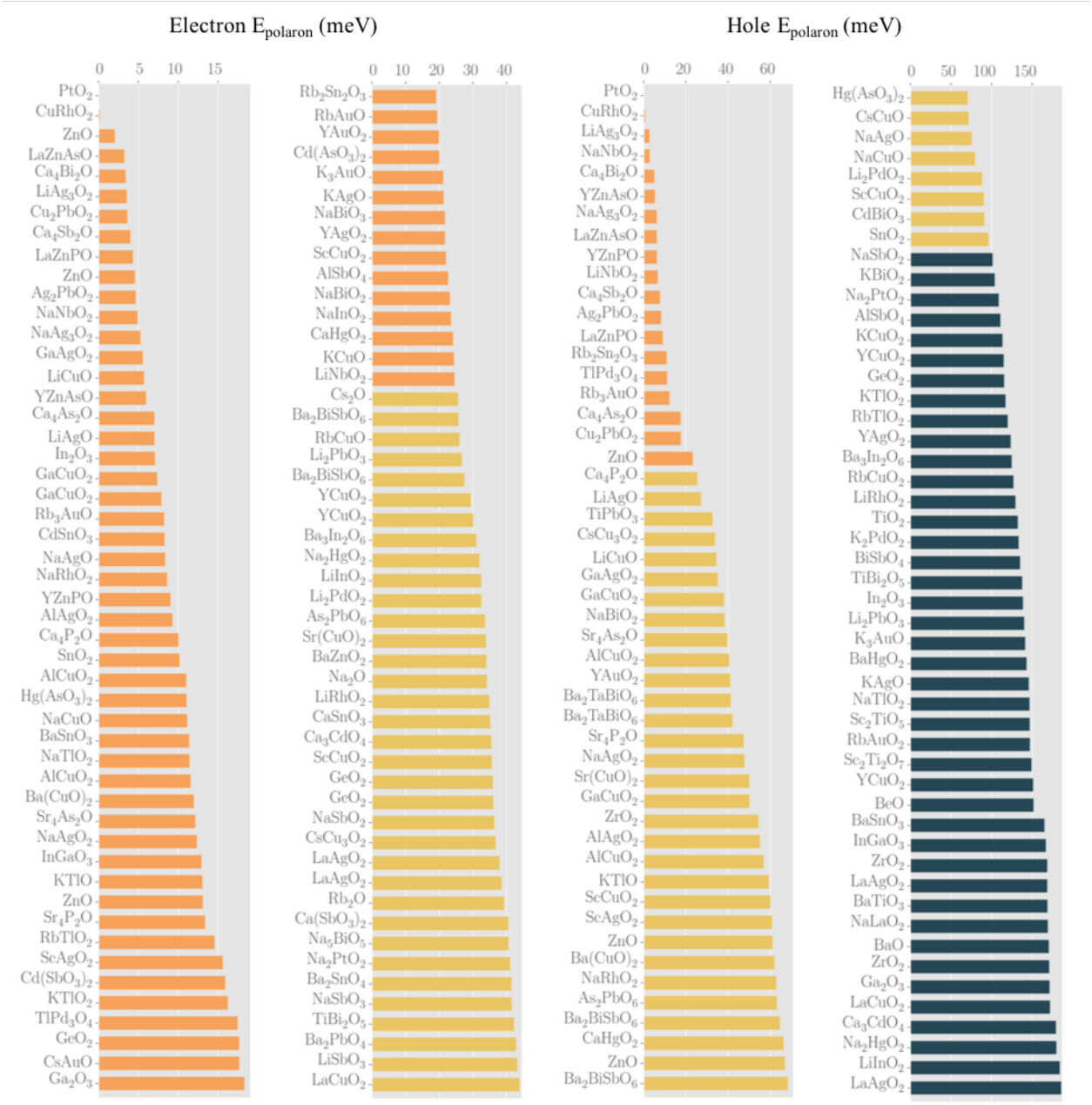

Figure S1: Electron and hole polaron binding energies calculated using the effective masses and dielectric constants from public data-sets. Some compositions have multiple entries due to polymorphism.

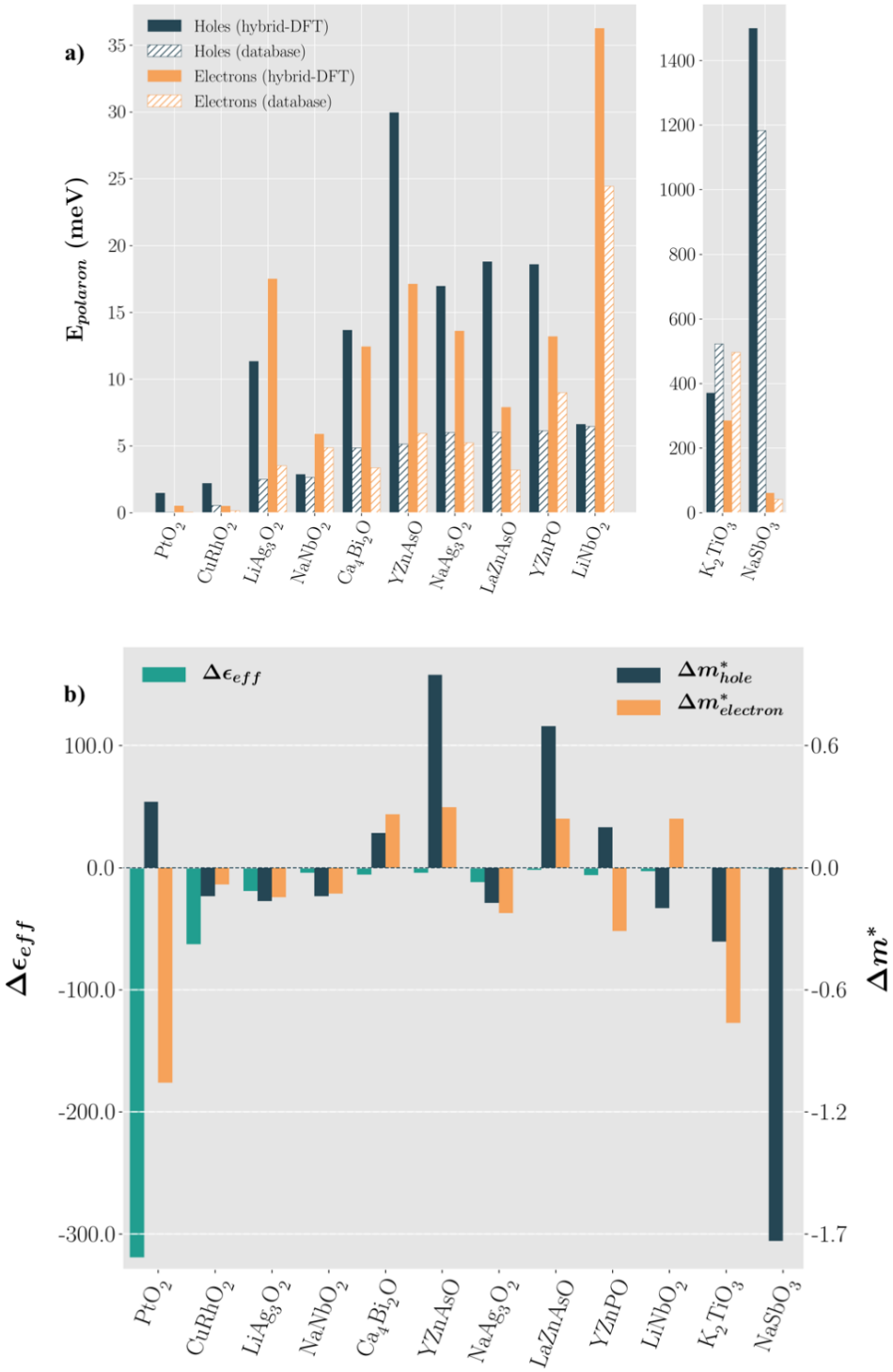

Figure S2: a) Polaron energy ($E_{polaron}$) values as calculated using hybrid-DFT (solid bars) and database (hatched bars) for electrons (orange bars) and holes (blue bars). b) Absolute difference (database derived minus Hybrid-DFT derived) in ϵ_{eff} (green bars) and effective mass (m^*) for electrons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

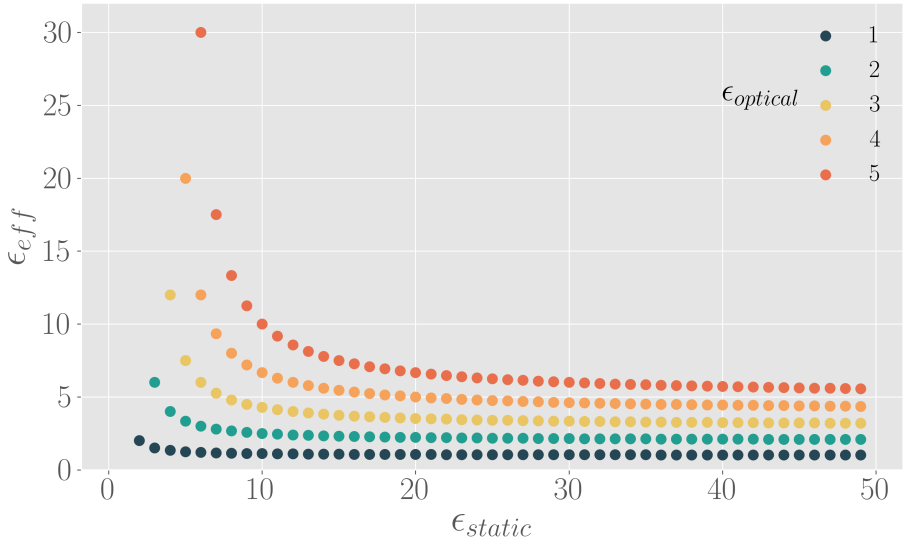

Figure S3: Visualization of the variation of ϵ_{eff} (y-axis) with ϵ_s (x-axis) at different fixed values of ϵ_∞. For $\epsilon_s > 20$ the system is in a strong screening regime where ϵ_{eff} shows little variation.