Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information

s valence electrons in cations of metal oxides serving as descriptors for electron and hole polarons

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For each material, we use supercell approach to calculate the polaron formation. As the lattice parameters are different, the details of the supercell are different. Here, we explain the calculation parameters required for each material individually.

We selected rutile TiO_2 with space group $I4_1/amd$ and V_2O_5 with space group pmmn for 2×2×1 and 3×3×3 cell expansion respectively. TiO_2 supercell parameters are a =10.62 Å, b =11.17 Å, c= 9.40 Å, α = β = γ = 90°, V_2O_5 supercell parameters are a =10.90 Å, b =14.26 Å, c= 11.55 Å, α = β = γ = 90°.We used supercells for subsequent calculations.

We used $SrTiO_3$ unit cell with space group P42/nmc for structural optimization, where a = b = c= 3.945 Å, α = β = γ = 90°. After the optimization is completed, we carry out 3×3×3 cell expansion, use supercell for electron polaron formation research.

We used ZrO_2 unit cell with space group $P4_2/nmc$ for calculation, where a=3.64Å, b=3.64Å, c=5.32Å, α=β=γ=90°. For the polarons calculations, we used a 3×3×2 supercell with 108 atoms. For MoO_3, we used primitive unit cells with a=3.76 Å, b=3.96 Å, c=14.43 Å, α=β=γ=90° for 3 × 3 × 1 cell expansion.

We selected HfO_2 primitive unit cells with a=b=4.86 Å, c =3.23 Å, α =γ =β =90° for 2×2×2 cell expansion. For Ta_2O_5 and $NaTaO_3$ we selected primitive unit cells with a=12.89 Å, b=4.87 Å, c =5.54 Å, α =γ =90°, β=104.3° and a=5.53 Å, b=5.59 Å, c =7.87 Å, α =γ =β =90° for 1×2×2 and 2×2×2 cell expansion and used the supercell containing

122 and 160 atoms for calculation.