

Computational Prediction of the Thermoelectric Performance of LaZnOP_n (P_n = P, As)

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Supplementary Information

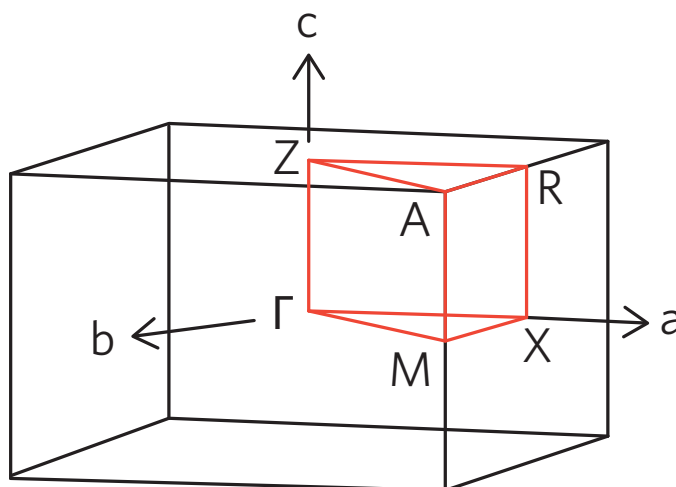


Figure S1: Brillouin zone of the $P4/nmm$ space group with the high symmetry points labelled.

Table S1: The elemental HSE06 relaxed reference energies, used to calculate the formation enthalpies of LaZnOP and LaZnOAs. In the case of P and As, the polymorph calculated with the lowest total energy was chosen. A 450 eV plane wave energy-cutoff was used for all systems, and a k -point mesh chosen such that the total energy was converged to within 0.01 eV atom⁻¹.

Element	k -points	Energy (eV atom ⁻¹)
La	13 13 13	-4.98
Zn	30 30 14	-1.26
O	2 2 2	-6.38
P (red)	4 3 2	-6.48
As (black)	8 3 6	-5.61

Table S2: The enthalpies of formation (ΔH_f) of LaZnOP and LaZnOAs, calculated using HSE06.

Compound	Total energy (eV)	ΔH_f (eV)
LaZnOP	-55.70	-8.75
LaZnOAs	-54.06	-8.81

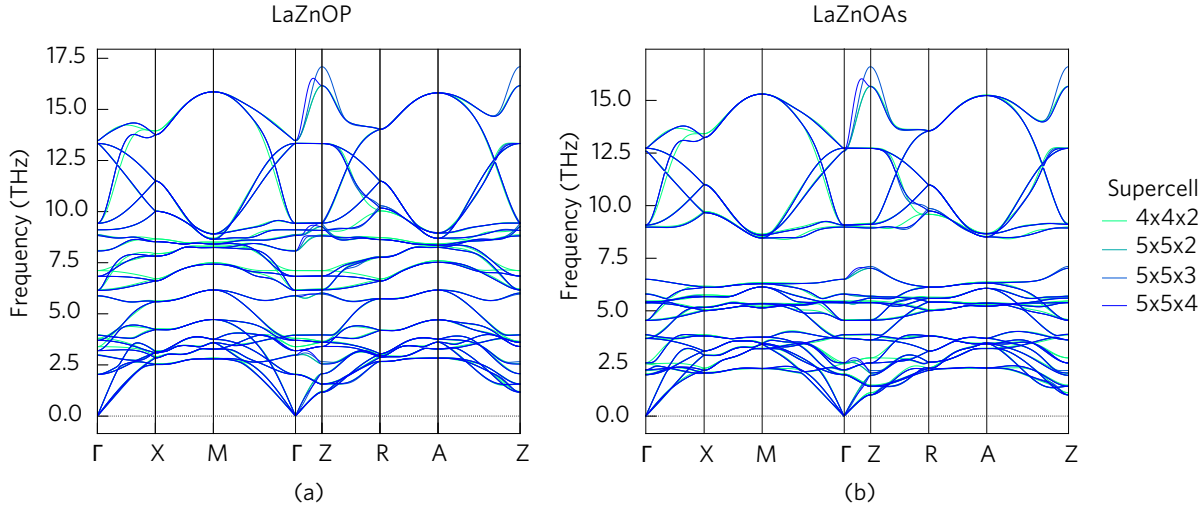


Figure S2: Convergence of phonon dispersion curve with supercell size for (a) LaZnOP and (b) LaZnOAs calculated using the PBEsol functional, plotted along a high symmetry pathway.

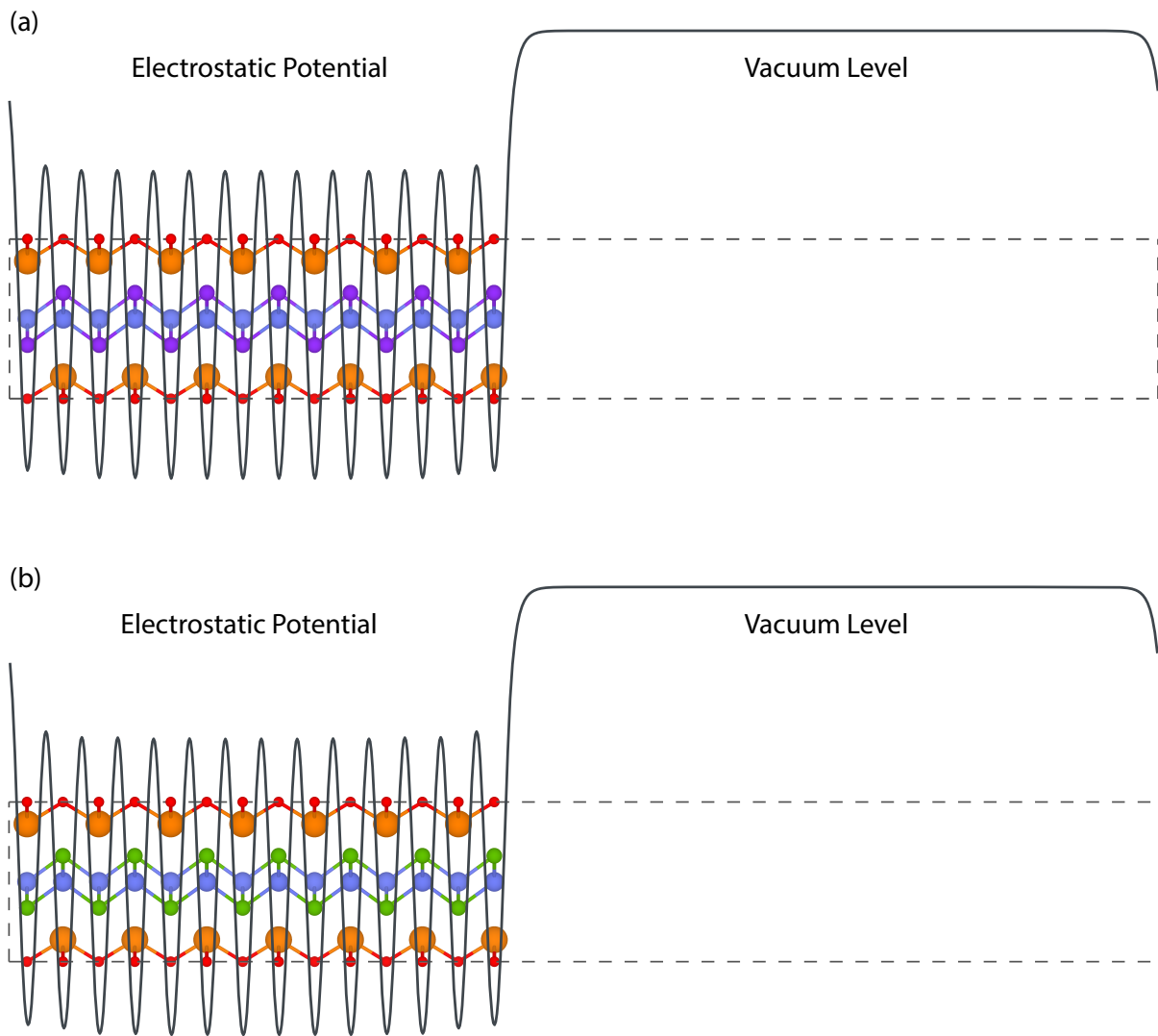


Figure S3: Slab model used to align the core electron eigenvalues to the vacuum level viewed along the (001) direction in (a) LaZnOP and (b) LaZnOAs. The blue line denotes the electrostatic potential calculated using HSE06+SOC. La, Zn, O and P and As atoms are shown in orange, grey, red, blue and green, respectively.

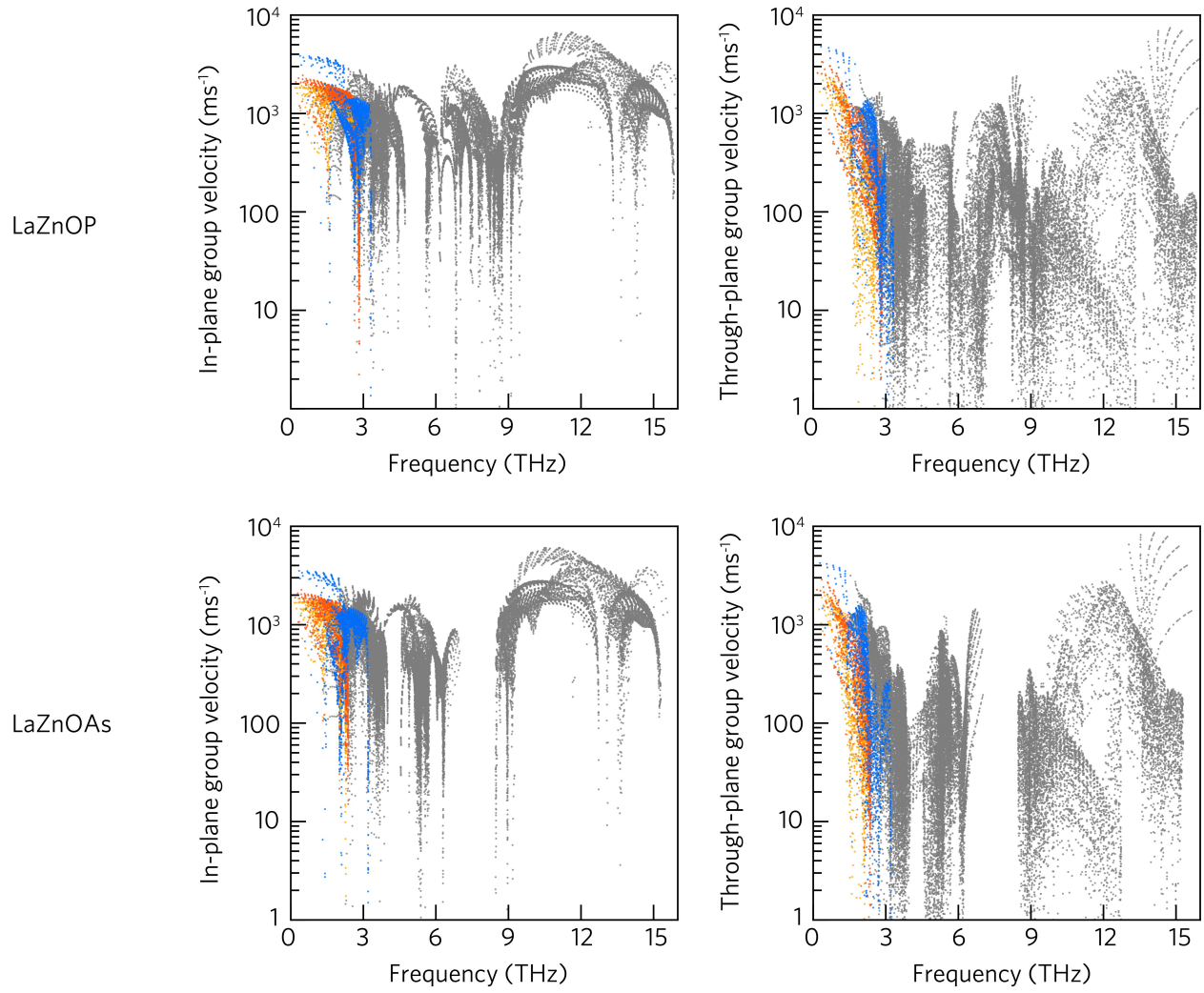


Figure S4: In-layer and through-layer phonon group velocities against frequency for LaZnOP and LaZnOAs at 300 K. The group velocities of the longitudinal acoustic mode is highlighted in blue, and the two transverse acoustic phonon modes are highlighted in orange and yellow, respectively.

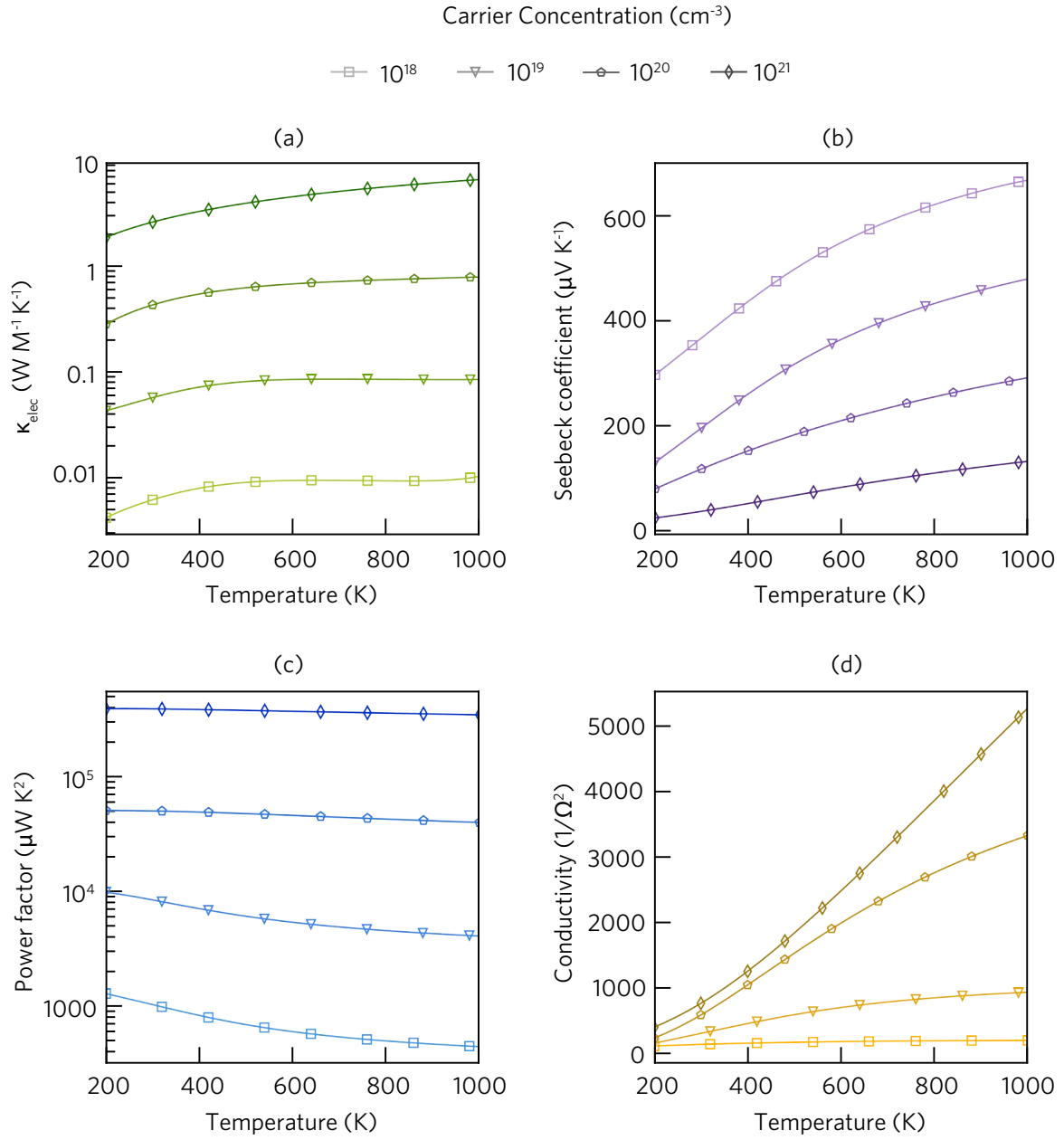


Figure S5: Plots of (a) electronic thermal conductivity, (b) Seebeck coefficient, (c) Power factor and (d) electrical conductivity against temperature plotted at various p-type carrier concentrations for LaZnOP, calculated using HSE06+SOC.

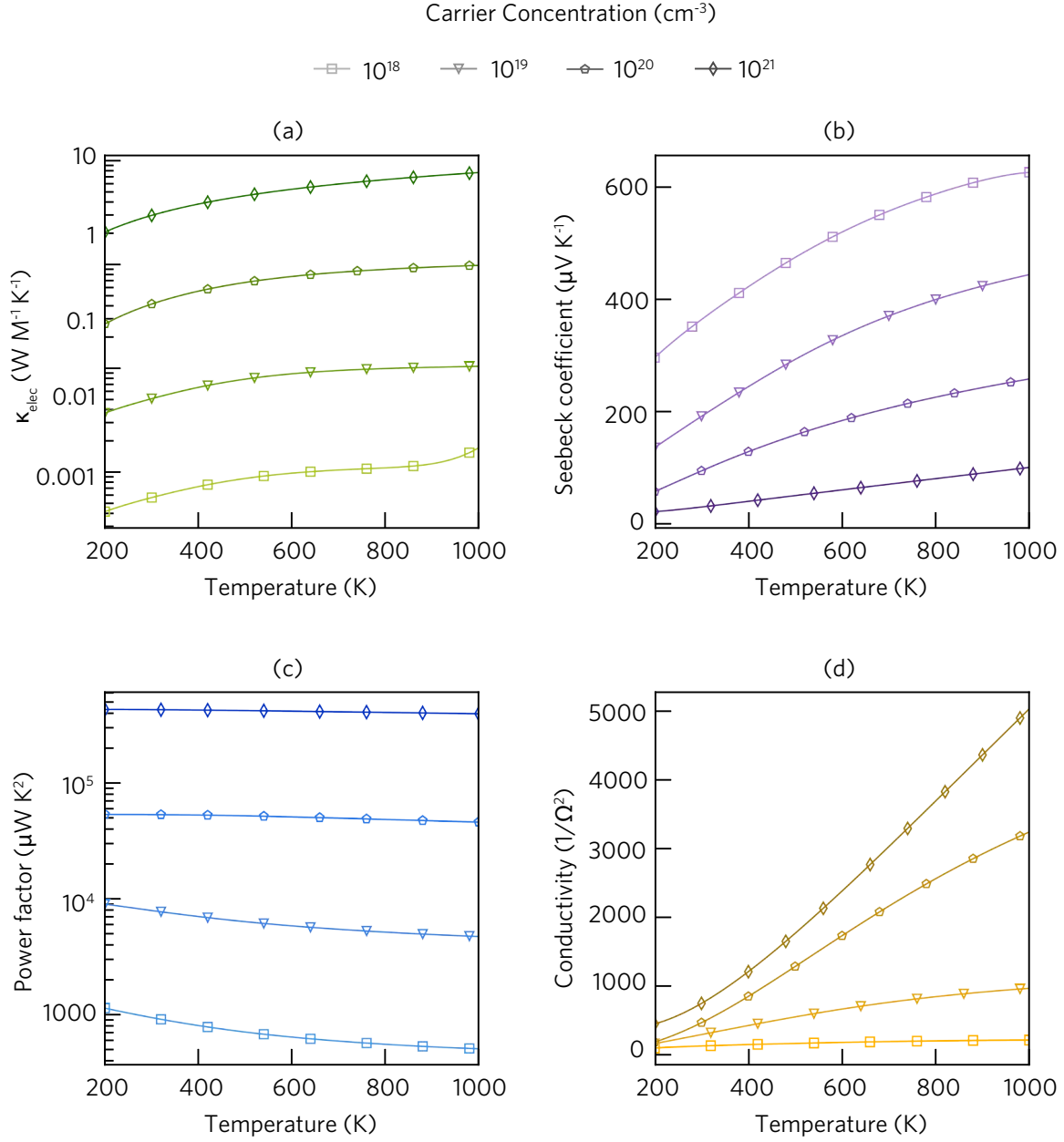


Figure S6: Plots of (a) electronic thermal conductivity, (b) Seebeck coefficient, (c) Power factor and (d) electrical conductivity against temperature plotted at various p-type carrier concentrations for LaZnOAs, calculated using HSE06+SOC.