Article

Predicting Interfacial Thermal Resistance by Ensemble Learning

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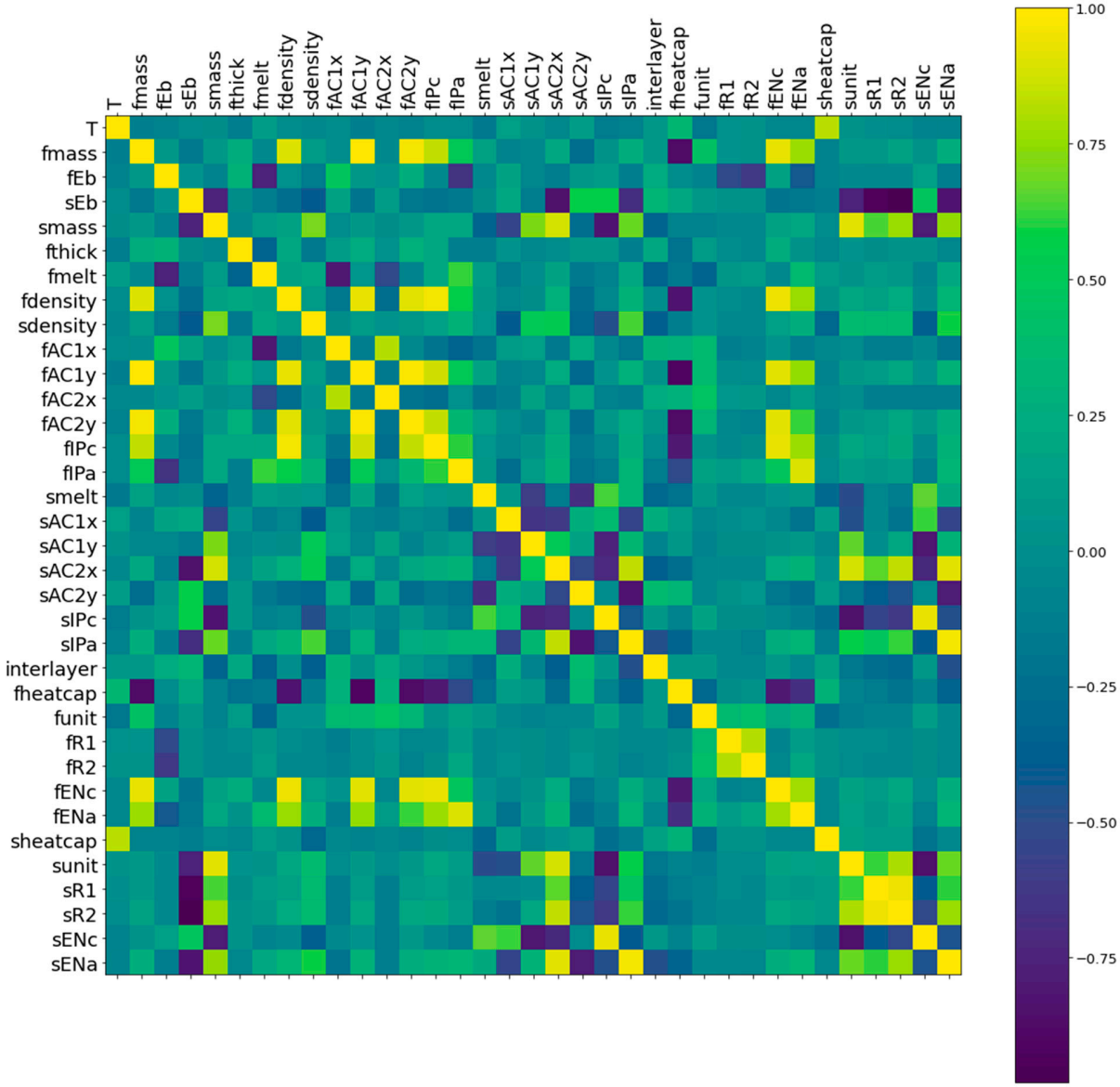

Figure S1. Pearson correlation coefficient map between all 35 descriptors in the raw dataset.

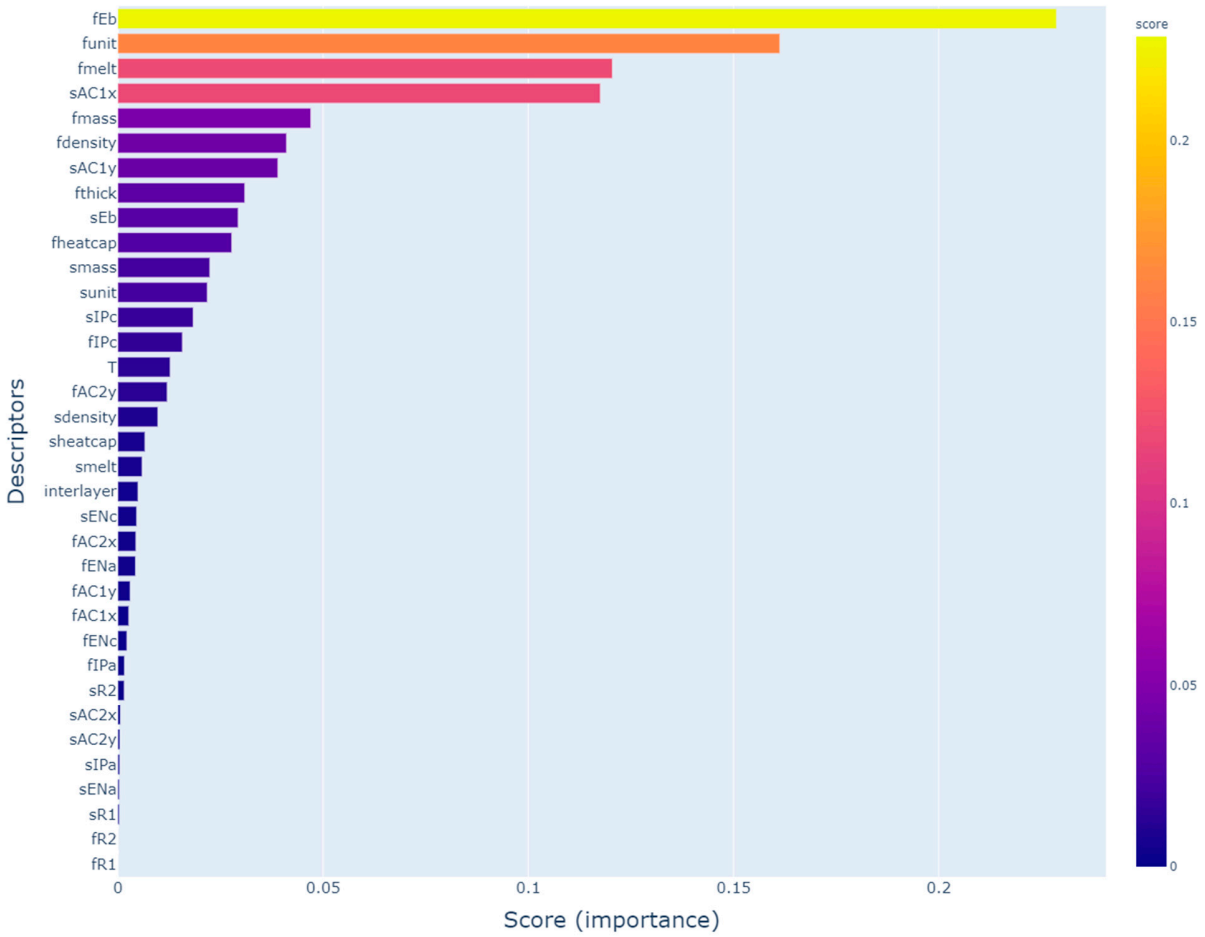

Figure S2. Rank of Descriptors based on importance score provided by XGB model.

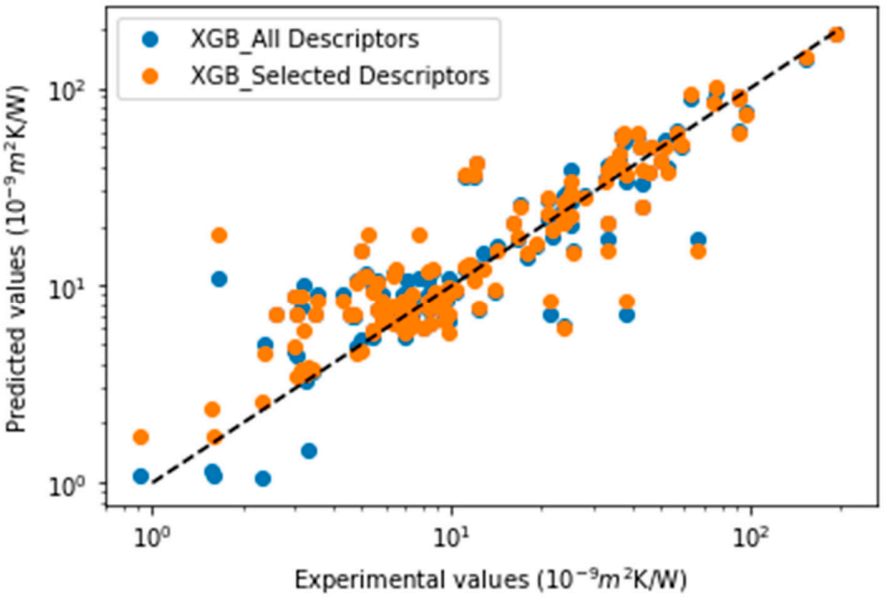

Figure S3. Correlation between the experimental values and values predicted by XGB model with all descriptors (blue dots) and selected descriptors (orange dots).

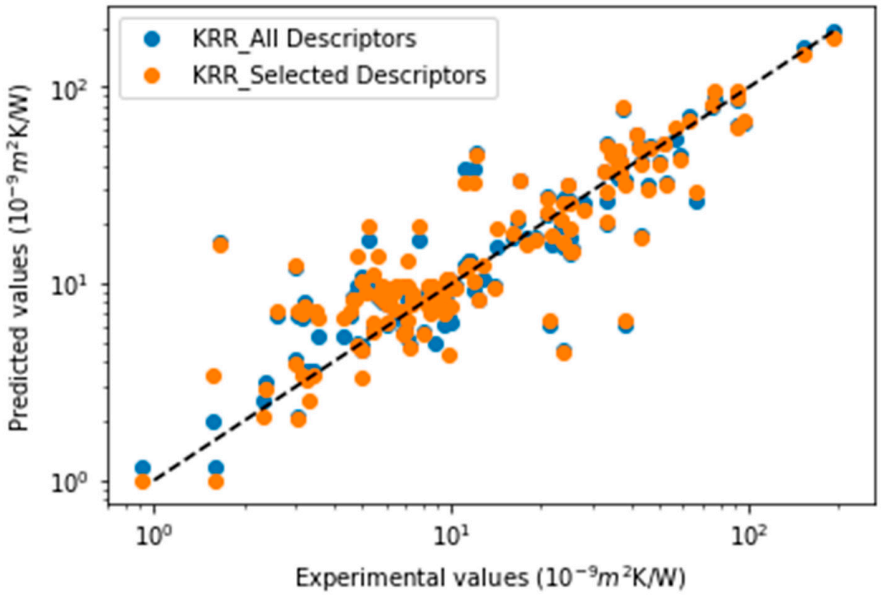

Figure S4. Correlation between the experimental values and values predicted by KRR model with all descriptors (blue dots) and selected descriptors (orange dots).

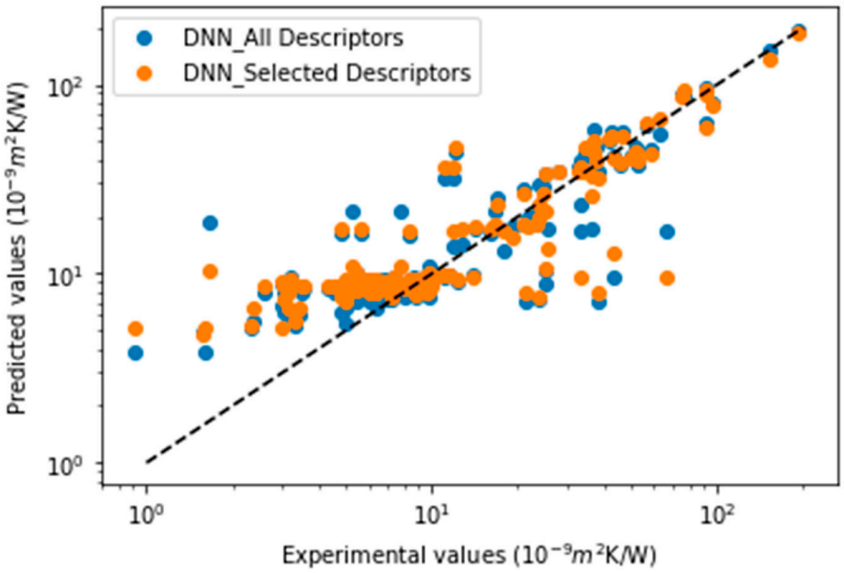

Figure S5. Correlation between the experimental values and values predicted by DNN model with all descriptors (blue dots) and selected descriptors (orange dots).

Table S1. Abbreviations of descriptors and the target explored in this work

Descriptor Abbreviation	Remarks
T	temperature (K)
fmass	film mass (u)
fEb	film binding energy (eV/f.u.)
sEb	substrate binding energy (eV/f.u.)
smass	substrate mass (u)
fthick	film thickness (nm)
fmelt	film melting point (K)
fdensity	film density (g/cm^3)
sdensity	substrate density (g/cm^3)
fAC1x, fAC1y, fAC2x, fAC2y	atomic coordinates for film [The group as the x coordinate and the period as the y coordinate as (ACix, ACiy), where i represents the order of the elements of the compound]
fIPc	film ionic potential for cation
fIPa	film ionic potential for anion
smelt	substrate melting point (K)
sAC1x, sAC1y sAC2x, sAC2y	atomic coordinates for substrate [The group as the x coordinate and the period as the y coordinate as (ACix, ACiy), where i represents the order of the elements of the compound]
sIPc	substrate ionic potential for cation
sIPa	substrate ionic potential for anion
fheatcap	film heat capacity (J/gK)
funit	film volume per formula unit (10^-29 m^3/f.u.)
sR1	atomic ratio of the first element of substrate
sR2	atomic ratio of the second element of substrate
sENc	substrate electronegativity for cation
sENa	substrate electronegativity for anion
itr	interfacial thermal resistance (m^2K/GW)

Table S2. Top 20 material systems with high ITR predicted by ensemble model

Material Systems	Predicted ITR by Ensemble Model
Bi/Diamond	65.67
Bi/Graphite	63.57
Bi/Graphene	63.34
Bi/S	55.66
Bi/P	55.38
Bi/B	51.53
PtS/Diamond	50.42
PtS/Graphene	48.97
Bi/HgO	48.89
PtS/Graphite	48.48
Ag2O/Diamond	48.04
Bi/BN	47.98
Bi/B2O3	47.96
Bi/HgS	47.57
Sn/Diamond	47.49
Bi/BeO	47.22
Ag2O/GaP	47.21
PdTe/Diamond	47.15
ZnS/Diamond	46.96
S/Diamond	46.75