Supplementary information to "Large-scale benchmark of exchange-correlation functionals for the determination of electronic band gaps of solids"

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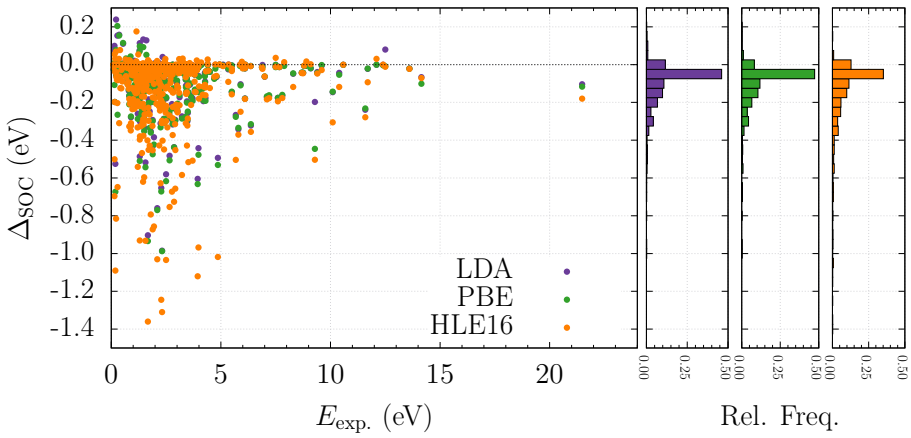

Figure S1: Spin-orbit coupling shift, $\Delta_{\mathrm{SOC}} = E_g^{\mathrm{SOC}} - E_g^{\mathrm{no\ SOC}}$ as a function of experimental gap, for LDA, PBE and HLE16. The corresponding histograms are also indicated for each distribution. No major qualitative differences distinguish the three functionals, but there are quantitative differences between HLE16 and LDA/PBE if we compare the mean value (LDA: -0.08 eV; PBE: -0.09 eV; HLE16: -0.14 eV) and the standard deviation of the distributions (LDA: 0.13 eV; PBE: 0.13 eV; HLE16: 0.22 eV). In specific cases the correction can double from LDA/PBE to HLE16, as mentioned in the main text.

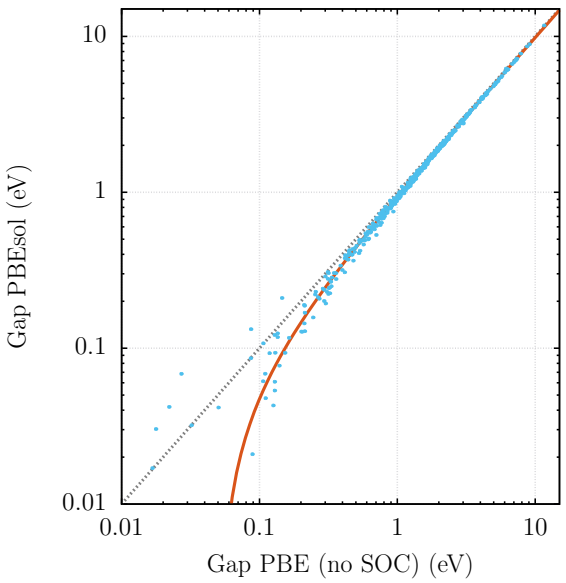

Figure S2: Dispersion of band gaps calculated with PBE vs. PBEsol, displayed in logarithmic scale. In orange, the linear fit $f(x) = a*x+b$ to this data, with $a = 0.9877$ and $b = -0.05155$. The line $y = x$ is added as a guide to the eye.

Figure S3: Mean absolute percentage error (in %) for the subsets of materials containing each element of the periodic table. Upper panel: LDA calculations. Lower panel: PBE calculations. Gray cases indicate that there are no materials containing the corresponding element.

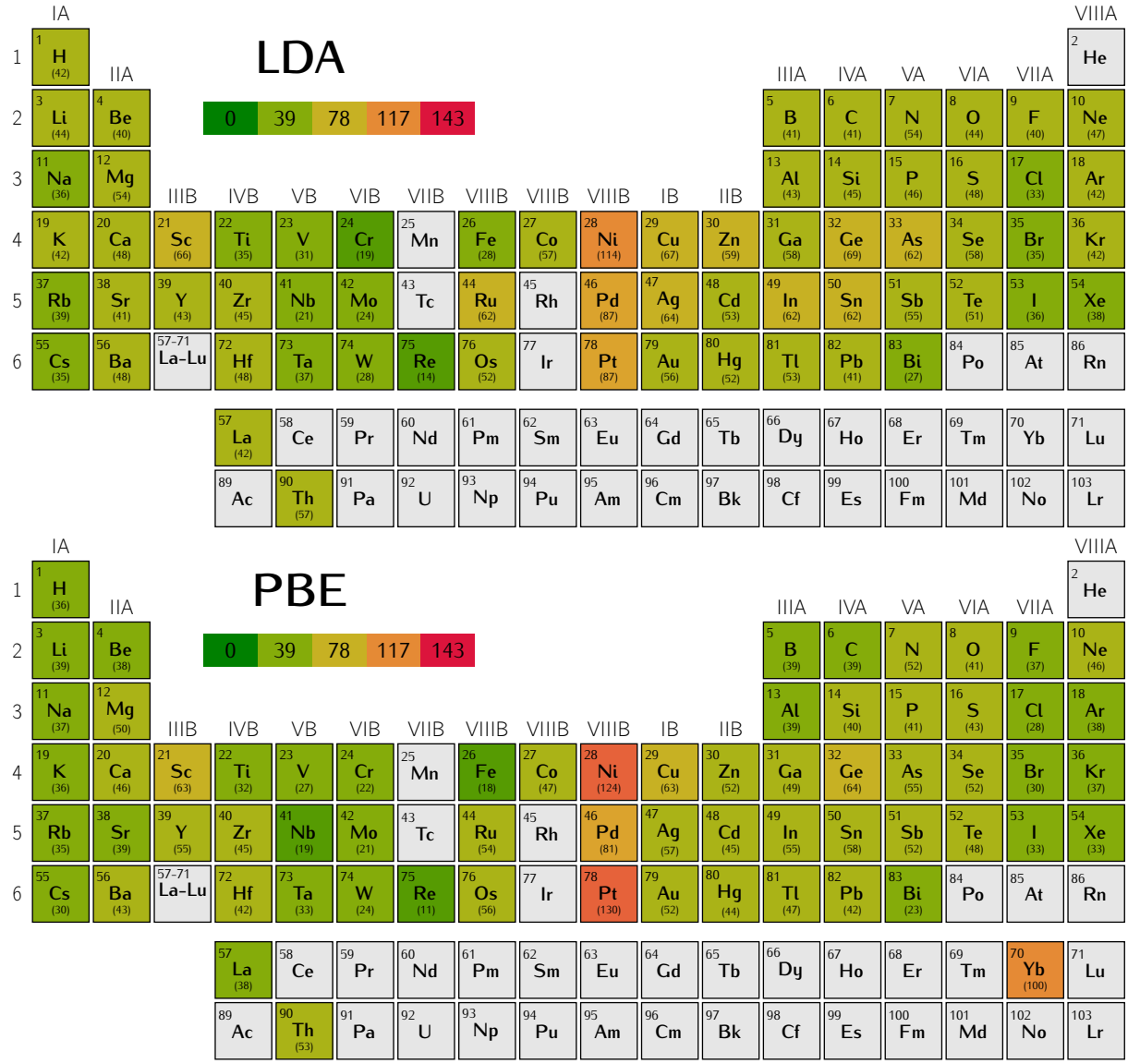

Figure S4: Mean absolute percentage error (in %) for the subsets of materials containing each element of the periodic table. Upper panel: HLE16 calculations without spin-orbit coupling. Lower panel: HLE16 calculations including spin-orbit coupling. Gray cases indicate that there are no materials containing the corresponding element.

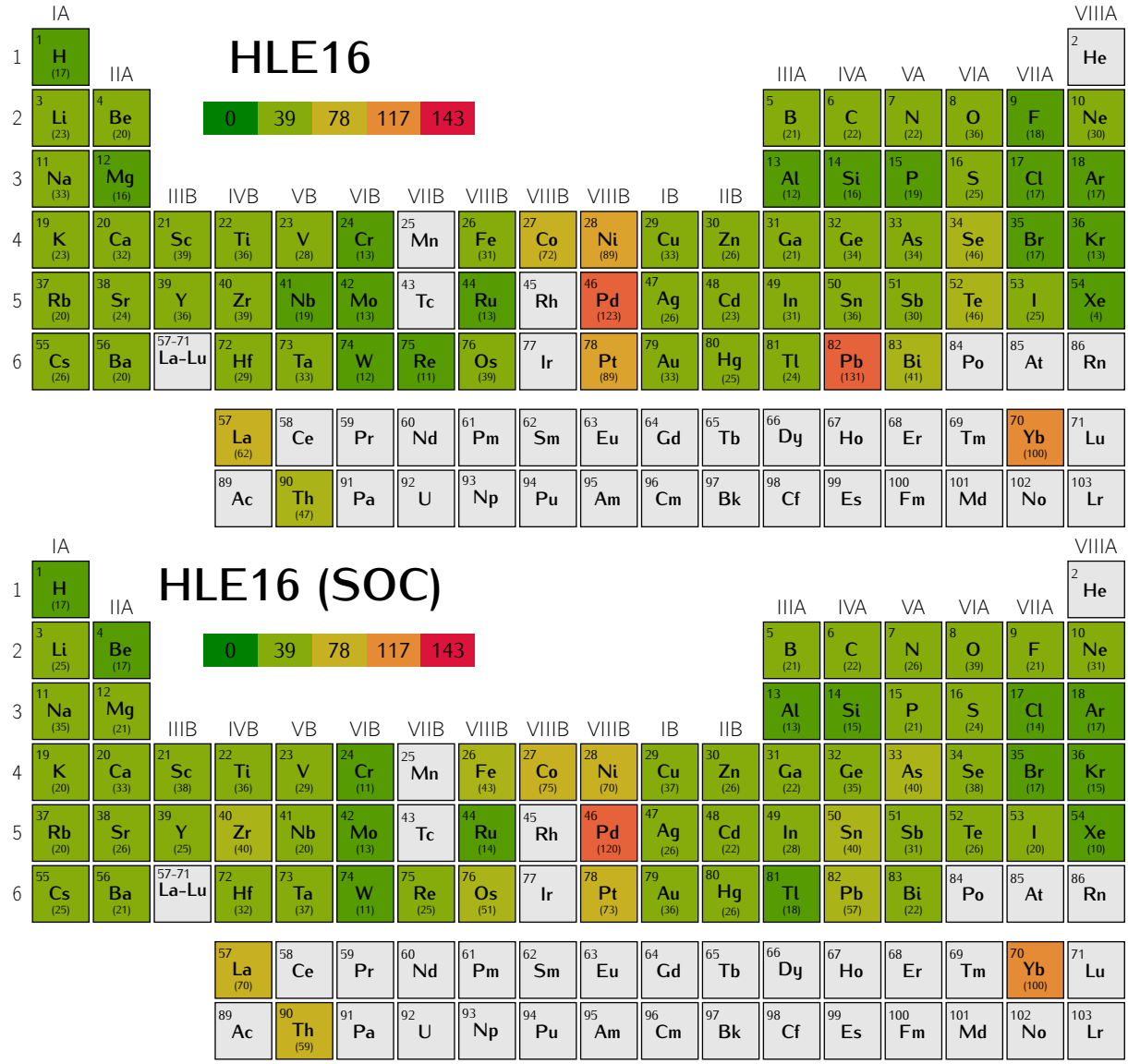

Figure S5: Mean absolute percentage error (in %) for the subsets of materials containing each element of the periodic table. Upper panel: MBJ calculations. Lower panel: HSE06 calculations. Gray cases indicate that there are no materials containing the corresponding element.

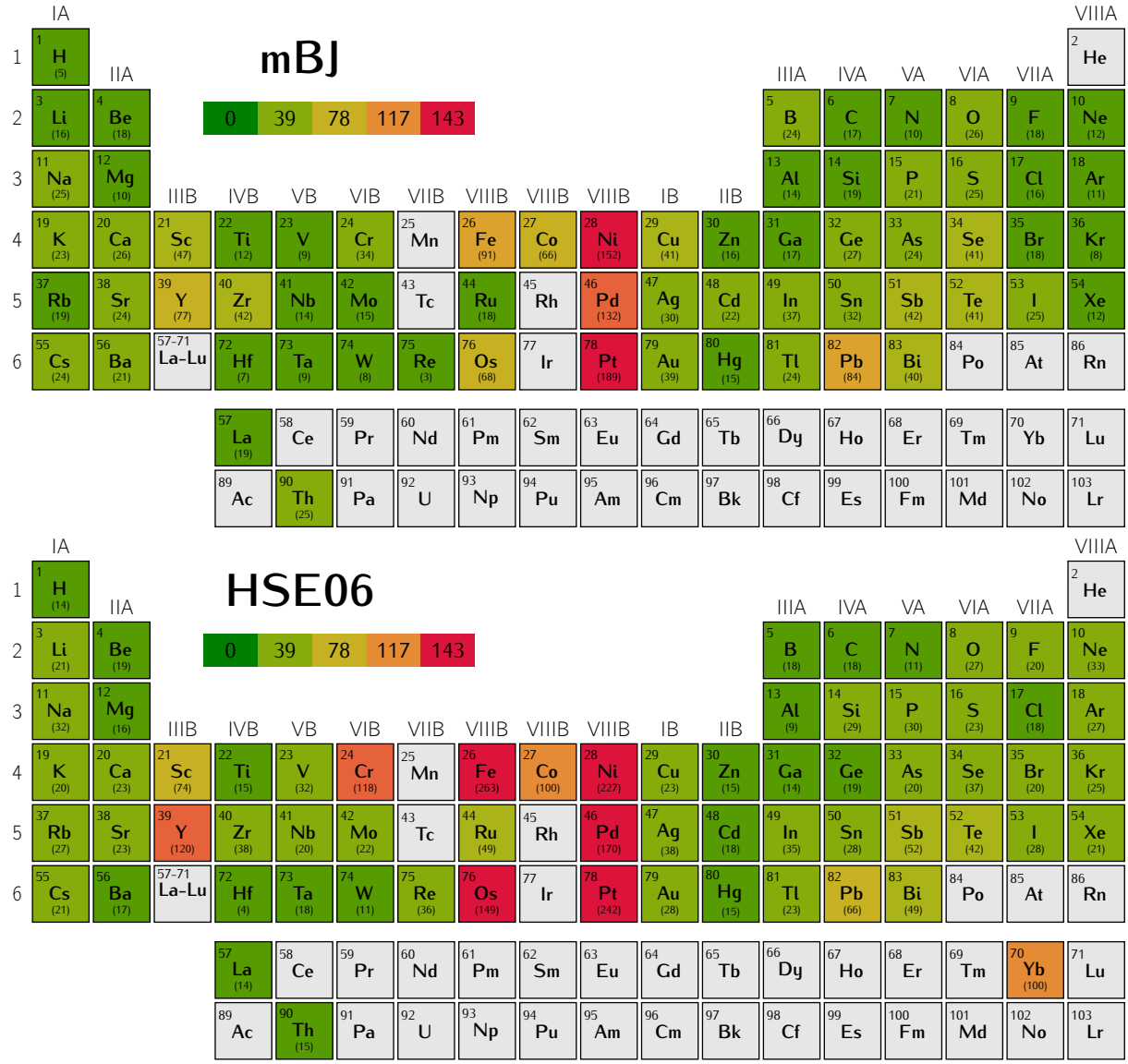

Figure S6: Mean absolute percentage error (in %) for the subsets of materials containing each element of the periodic table. Upper panel: HSE_{mix} calculations. Lower panel: PBE0 calculations. Gray cases indicate that there are no materials containing the corresponding element.

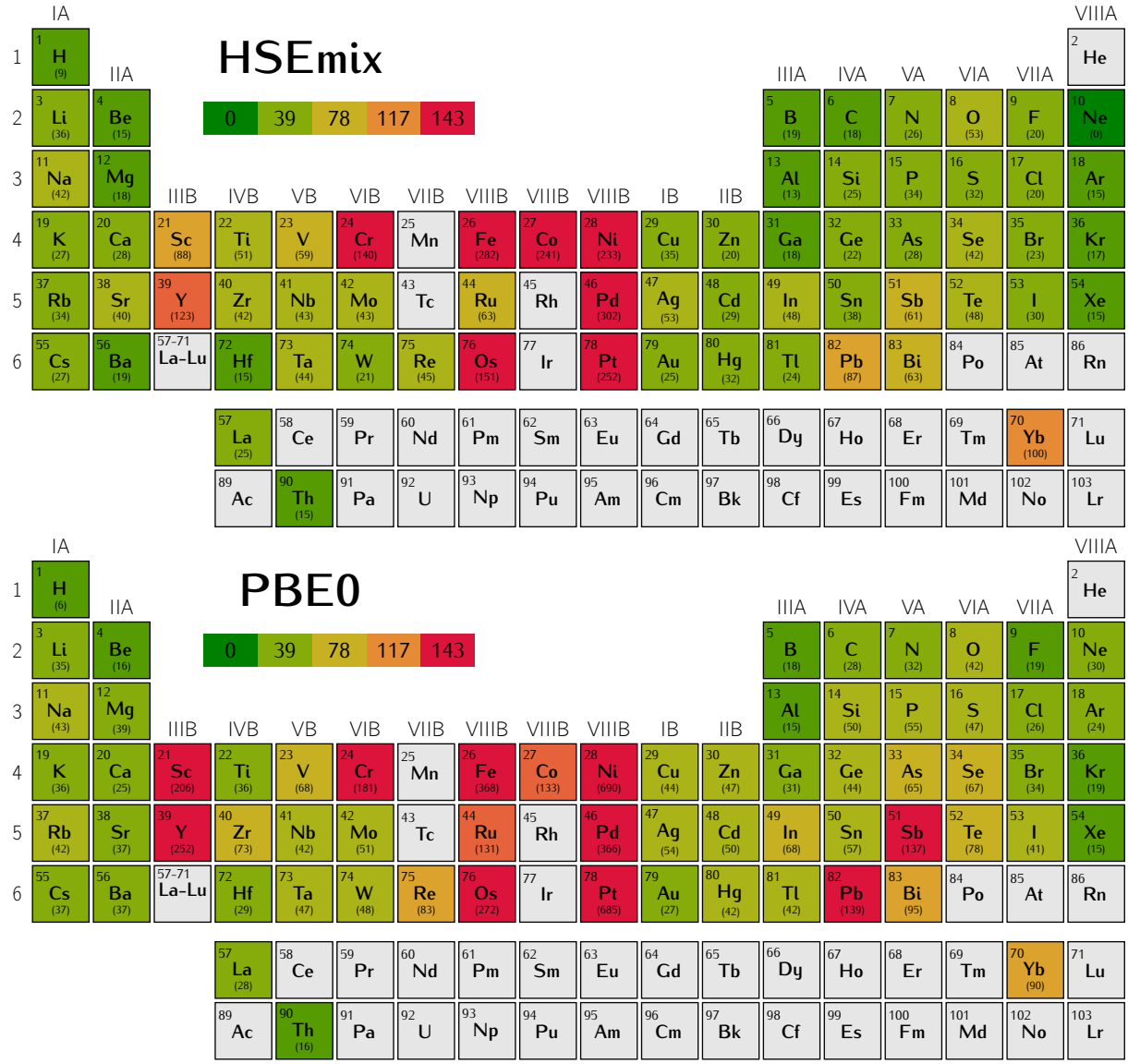

Figure S7: Mean absolute percentage error (in %) for the subsets of materials containing each element of the periodic table. $PBE0_{mix}$ calculations. Gray cases indicate that there are no materials containing the corresponding element.

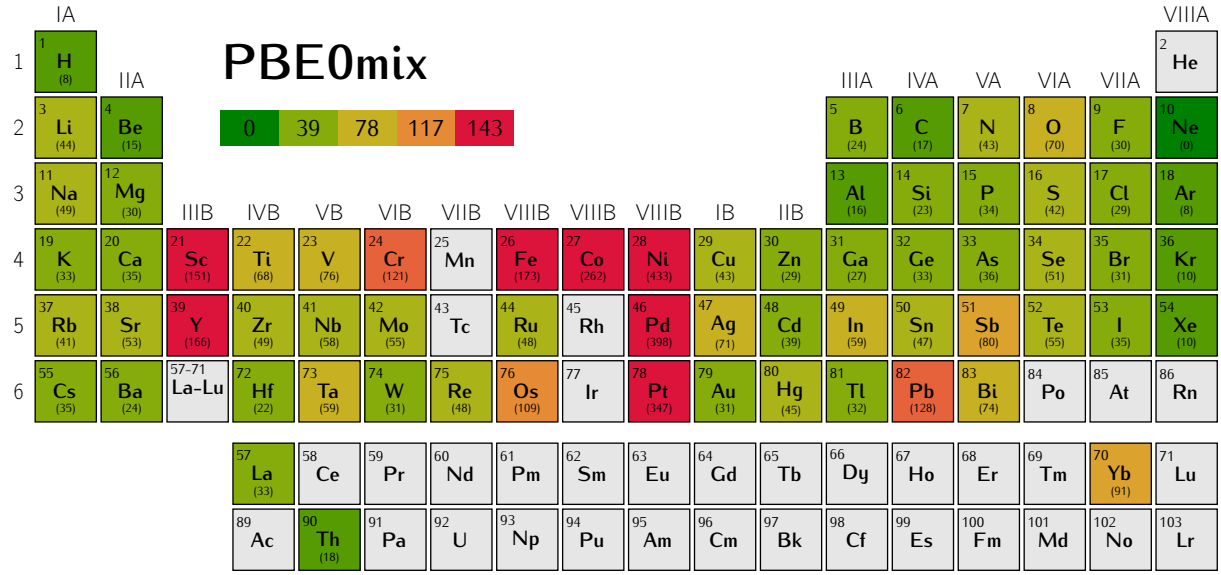

Figure S8: Histograms of MAPE and MPE for different functionals considered in this work as a function of the experimental band gap size. Due to the fact that few entries have band gap larger than 10 eV, all systems satisfying this condition are collected in one group.

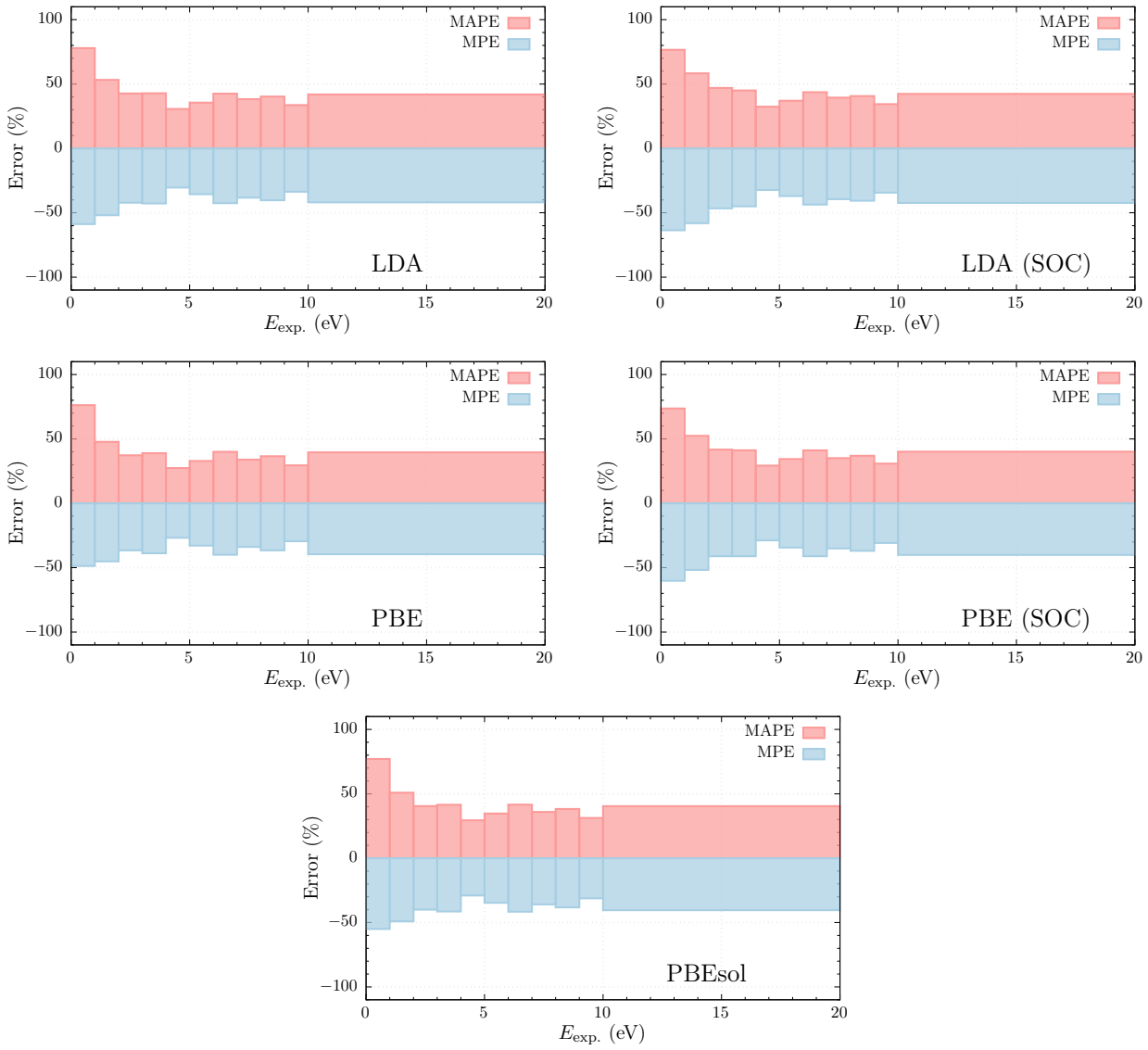

Figure S8: (cont.) Histograms of MAPE and MPE for different functionals considered in this work as a function of the experimental band gap size. Due to the fact that few entries have band gap larger than 10 eV, all systems satisfying this condition are collected in one group.

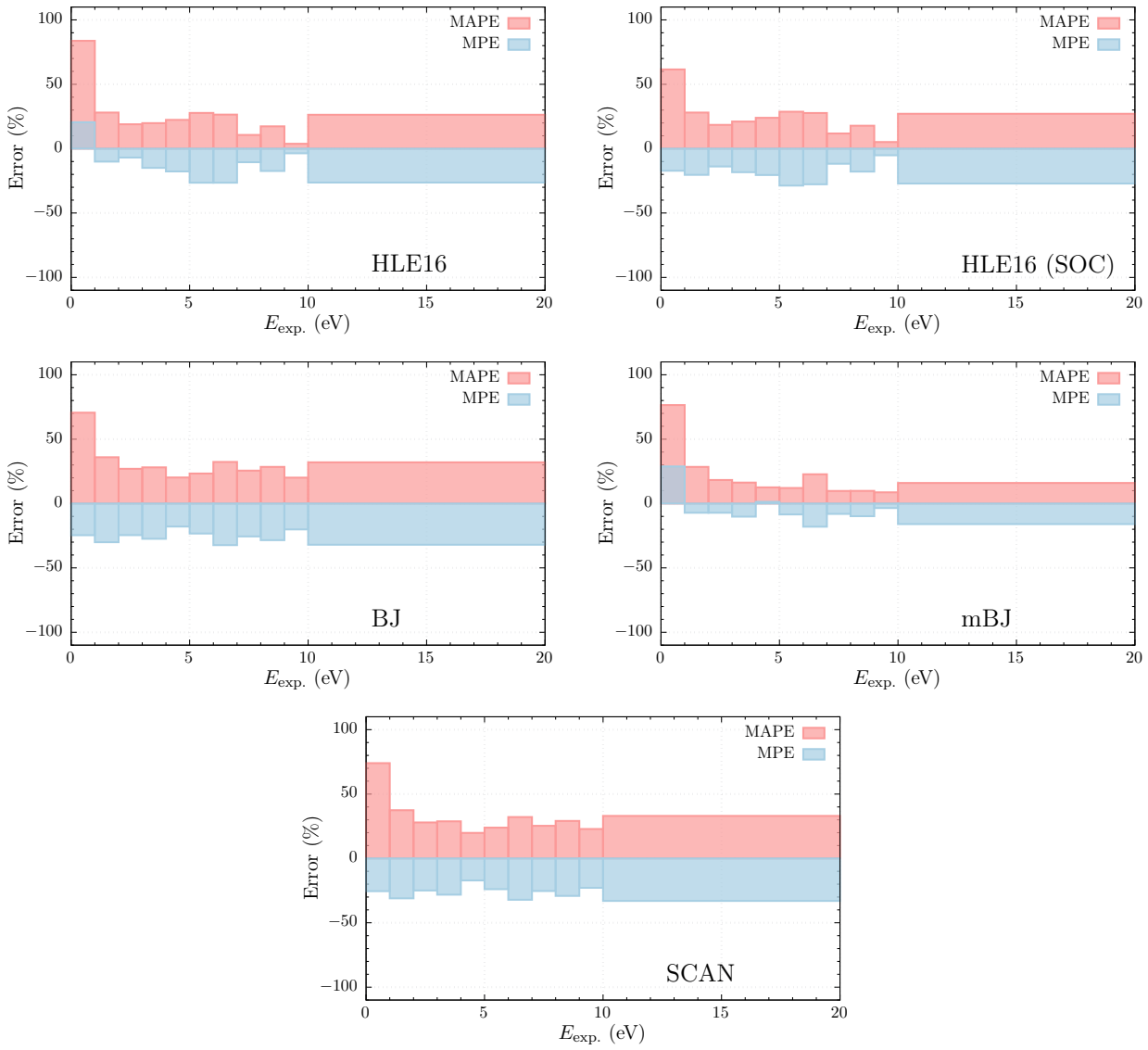

Figure S8: (cont.) Histograms of MAPE and MPE for different functionals considered in this work as a function of the experimental band gap size. Due to the fact that few entries have band gap larger than 10 eV, all systems satisfying this condition are collected in one group.

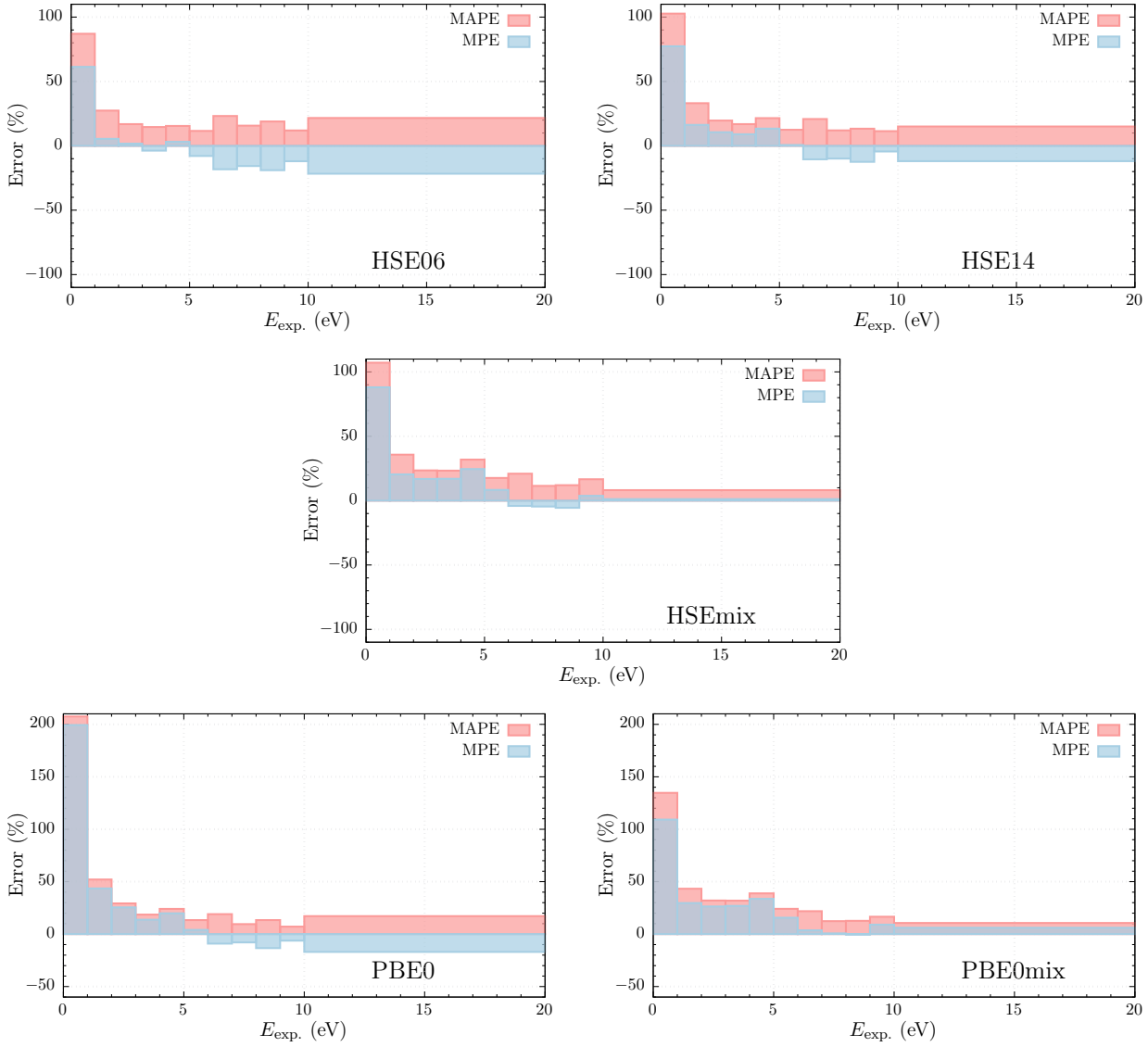

Table SI: Values of p obtained with the Wilcoxon signed-rank test for the absolute errors of each pair of functionals studied here. Due to the symmetry of the matix only the upper triangular part is shown. To improve readability, the statistic values W are not presented.

	LDA	LDA (SOC)	PBE	PBE (SOC)	PBEsol	HLE16	HLE16 (SOC)	BJ	mBJ	SCAN	HSE06	HSE14	HSE_{mix}	PBE0	$PBE0_{mix}$
LDA	—	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LDA (SOC)		—	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PBE			—	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PBE (SOC)				—	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PBEsol					—	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HLE16						—	0.00	0.00	0.02	0.00	0.14	0.89	0.01	0.00	0.00
HLE16 (SOC)							—	0.00	0.02	0.00	0.21	0.90	0.03	0.00	0.00
BJ								—	0.00	0.03	0.00	0.00	0.00	0.89	0.88
mBJ									—	0.00	0.36	0.00	0.00	0.00	0.00
SCAN										—	0.00	0.00	0.00	0.66	0.60
HSE06											—	0.00	0.00	0.00	0.00
HSE14												—	0.00	0.00	0.00
$HSE06_{mix}$													—	0.00	0.00
PBE0														—	0.05
$PBE0_{mix}$															—

Table SII: Values of p obtained with the Wilcoxon signed-rank test for the absolute percentage errors of each pair of functionals studied here. Due to the symmetry of the matix only the upper triangular part is shown. To improve readability, the statistic values W are not presented.

	LDA	LDA (SOC)	PBE	PBE (SOC)	PBEsol	HLE16	HLE16 (SOC)	BJ	mBJ	SCAN	HSE06	HSE14	HSE_{mix}	PBE0	$PBE0_{mix}$
LDA	—	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LDA (SOC)		—	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PBE			—	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.19	0.00
PBE (SOC)				—	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
PBEsol					—	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00
HLE16						—	0.00	0.00	0.21	0.00	0.13	0.32	0.00	0.00	0.00
HLE16 (SOC)							—	0.00	0.46	0.00	0.19	0.22	0.00	0.00	0.00
BJ								—	0.00	0.10	0.00	0.00	0.02	0.00	0.04
mBJ									—	0.00	0.86	0.00	0.00	0.00	0.00
SCAN										—	0.00	0.00	0.00	0.00	0.19
HSE06											—	0.00	0.00	0.00	0.00
HSE14												—	0.00	0.00	0.00
$HSE06_{mix}$													—	0.00	0.00
PBE0														—	0.00
$PBE0_{mix}$															—