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Article

Supplementary Material: Regression Machine-Learning Models Used to Predict DFT Computed NMR Parameters of Zeolites

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1. Table containing the Zeolite names as reported in the IZA [1] and the DFT optimized crystallographic lattice vectors.

Table S1. Zeolite names as reported in IZA and the DFT optimized crystallographic lattice vectors in Å.

Zeolite	a1	a2	a3	b1	b2	b3	c1	c2	c3
*MFI-TPA	19.727	0.000	0.000	0.000	13.315	0.000	0.000	0.000	19.862
MFI_F_ETPA_direct1	19.670	0.000	0.000	0.000	13.299	0.000	0.000	0.000	19.749
MFI_F_ETPA_direct2	19.520	0.000	0.000	0.000	13.287	0.000	0.000	0.000	19.789
MFI_F_ETPA_zigzag1	19.693	0.000	0.000	0.000	13.278	0.000	0.000	0.000	19.805
MFI_F_ETPA_zigzag2	19.724	0.000	0.000	0.000	13.326	0.000	0.000	0.000	19.701
ZSM-5_1	19.872	0.000	0.000	0.000	12.987	0.000	0.000	0.000	19.713
ZSM-5_2	19.822	0.000	0.000	0.000	12.974	0.000	0.000	0.000	19.673
ZSM-5_3	19.794	0.000	0.000	0.000	12.996	0.000	0.000	0.000	19.698
ZSM-5_4	19.881	0.000	0.000	0.000	12.984	0.000	0.000	0.000	19.701
ZSM-5_5	19.937	0.000	0.000	0.000	12.944	0.000	0.000	0.000	19.685
ZSM-5_6	19.866	0.000	0.000	0.000	12.919	0.000	0.000	0.000	19.701
ZSM-5_8	19.832	0.000	0.000	0.000	12.948	0.000	0.000	0.000	19.765
ZSM-5_9	19.760	0.000	0.000	0.000	12.887	0.000	0.000	0.000	19.875
ZSM-5_10	19.739	0.000	0.000	0.000	12.963	0.000	0.000	0.000	19.861
ZSM-5_12	19.825	0.000	0.000	0.000	12.937	0.000	0.000	0.000	19.815
ZSM-5_13	19.908	0.000	0.000	0.000	12.969	0.000	0.000	0.000	19.698
ZSM-5_14	19.819	0.000	0.000	0.000	12.949	0.000	0.000	0.000	19.698
ZSM-5_15	19.778	0.000	0.000	0.000	13.004	0.000	0.000	0.000	19.736
ZSM-5_16	19.854	0.000	0.000	0.000	13.020	0.000	0.000	0.000	19.698
ZSM-5_17	19.928	0.000	0.000	0.000	12.968	0.000	0.000	0.000	19.680
ZSM-5_18	19.853	0.000	0.000	0.000	12.913	0.000	0.000	0.000	19.691
ZSM-5_19	19.893	0.000	0.000	0.000	12.945	0.000	0.000	0.000	19.798
ZSM-5_20	19.920	0.000	0.000	0.000	12.926	0.000	0.000	0.000	19.728
ZSM-5_21	19.824	0.000	0.000	0.000	12.879	0.000	0.000	0.000	19.828
ZSM-5_22	19.749	0.000	0.000	0.000	12.960	0.000	0.000	0.000	19.840
ZSM-5_23	19.884	0.000	0.000	0.000	12.936	0.000	0.000	0.000	19.745
ZSM-5_24	20.117	0.000	0.000	0.000	12.804	0.000	0.000	0.000	19.591
*ify	15.508	0.000	0.000	0.000	15.508	0.000	0.000	0.000	11.090

Table S1. continuation of the table.

Zeolite	a1	a2	a3	b1	b2	b3	c1	c2	c3
*imf	7.224	28.362	0.000	-7.224	28.362	0.000	0.000	0.000	19.401
oko-cok-14	12.267	7.010	0.172	-12.267	7.010	-0.172	-4.029	0.000	11.493
*rro	7.350	0.000	0.012	0.000	8.734	0.000	-6.815	0.000	15.522
rwr	-3.968	3.968	13.894	3.968	-3.968	13.894	3.968	3.968	-13.894
sillimanite	7.681	0.000	0.000	0.000	5.823	0.000	0.000	0.000	7.497
*stf	6.977	9.290	-0.087	-6.977	9.290	0.087	-1.246	0.000	7.400
uov	12.382	0.000	0.000	0.000	11.138	19.376	0.000	-11.138	19.376
MFI-BT-P1	20.023	0.000	0.000	0.000	19.912	0.000	0.000	-0.136	13.417
MFI_TPAF_HT_monoclinique	19.876	-0.001	0.008	-0.001	20.154	0.000	0.006	0.000	13.329
*TON	10.737	0.009	0.153	0.013	9.923	-0.003	2.811	-0.047	10.836
*ITW	8.577	3.232	0.155	0.114	9.008	0.184	-1.818	1.601	8.318
*CHA	9.217	-0.601	-0.087	0.174	9.233	-0.137	-0.880	-0.764	9.359
AST-TMA	8.720	-0.034	0.033	-0.034	8.816	-0.020	0.049	-0.030	13.608
*AST	0.000	6.968	6.968	6.968	0.000	6.968	6.968	6.968	0.000

* zeolites, for which experimental ^{29}Si chemical shifts are collected (see main text).

2. Supporting figures

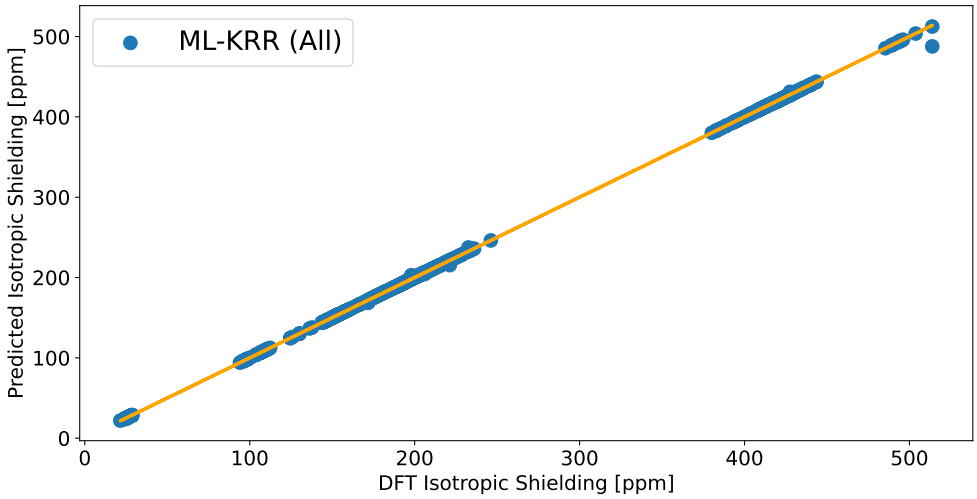

Figure S1. Predicted vs DFT isotropic shielding of all atoms in zeolites obtained with ML-KRR model.

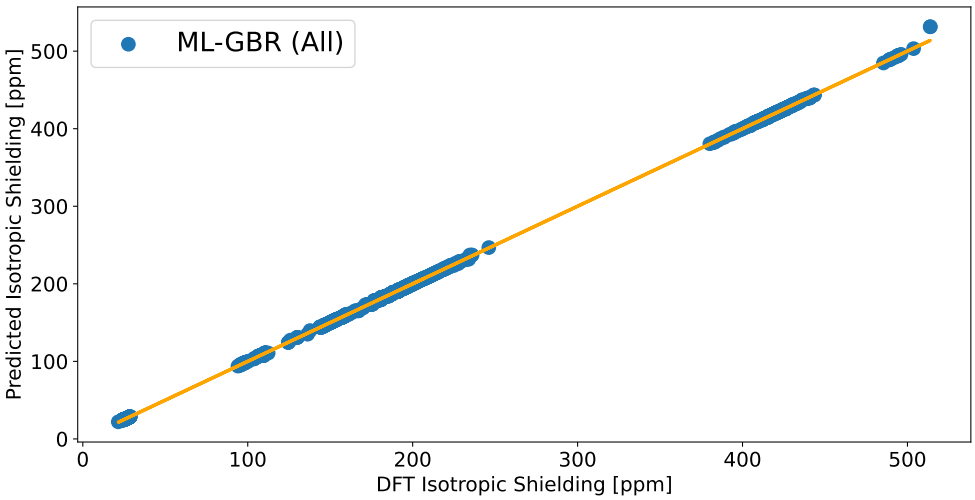

Figure S2. Predicted vs DFT isotropic shielding of all atoms in zeolites obtained with ML-GBR model.

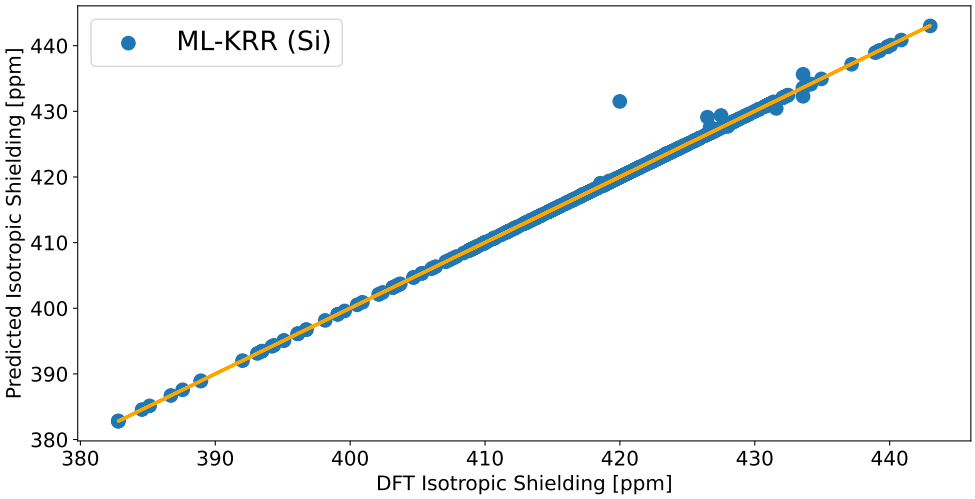

Figure S3. Predicted vs DFT isotropic shielding of Si atoms in zeolites obtained with ML-KRR model.

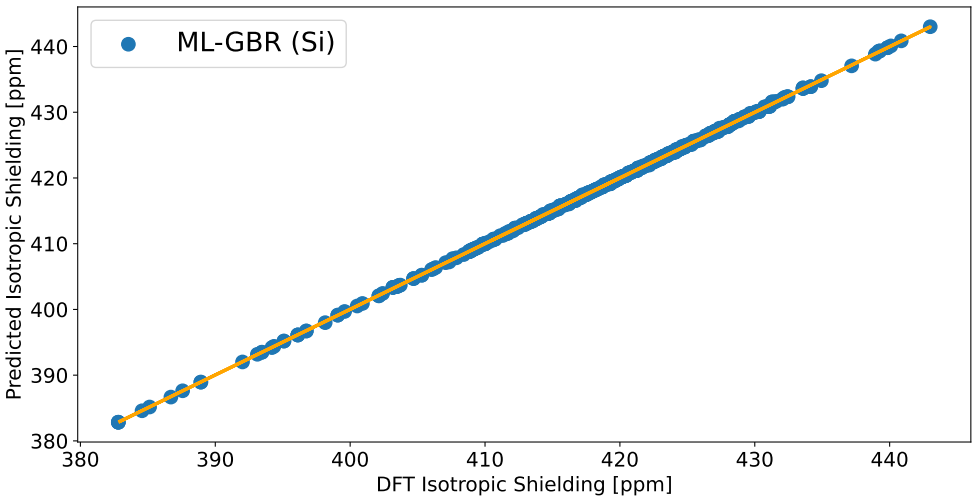

Figure S4. Predicted vs DFT isotropic shielding of Si atoms in zeolites obtained with ML-GBR model.

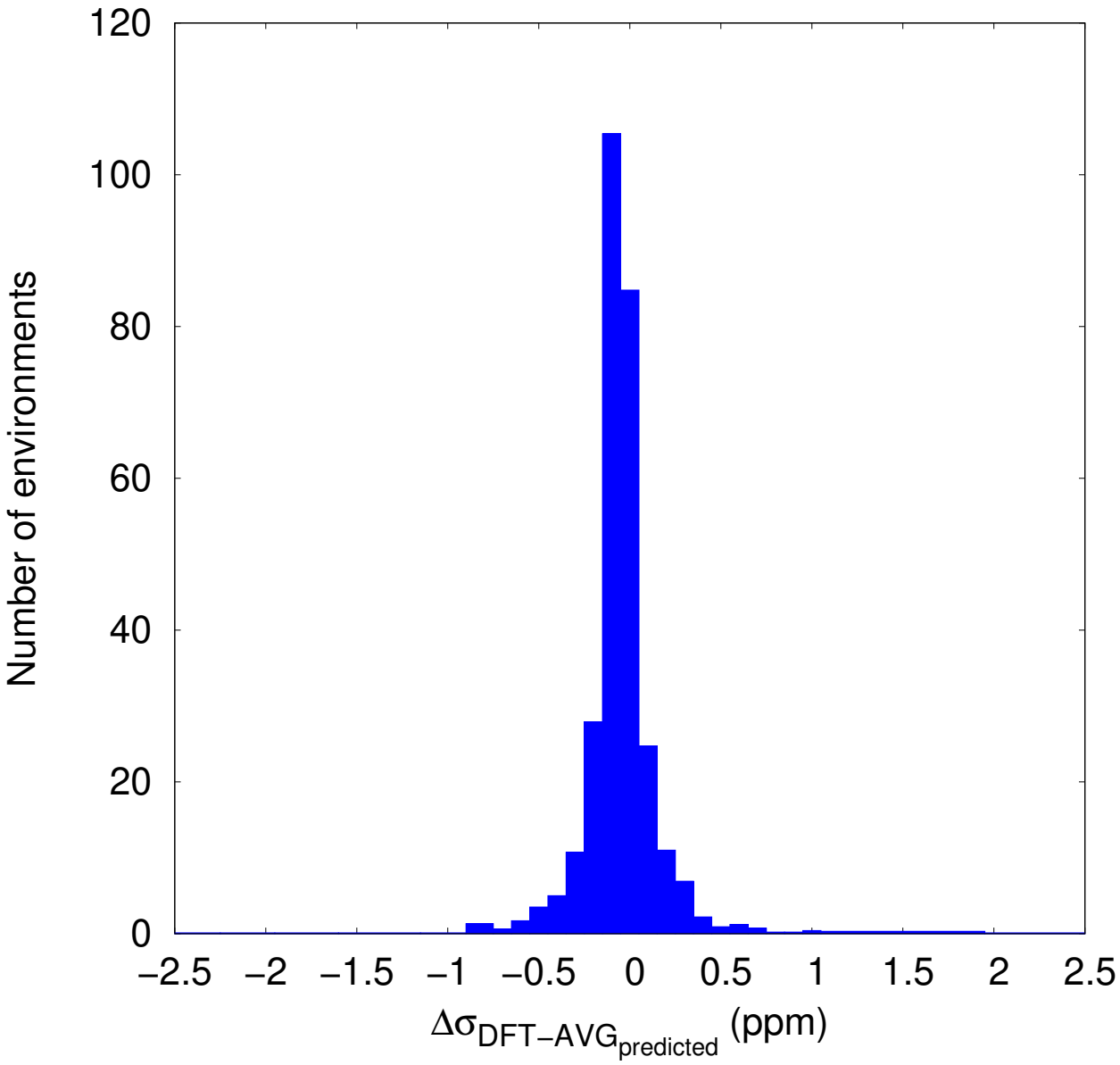

Figure S5. Distribution of the differences between the isotropic shielding values computed with DFT and the average between the predicted ML-KRR and ML-GBR values. All atomic environments are considered. The histograms are obtained with an interval of 0.1 ppm in the count of the number of atomic environments.

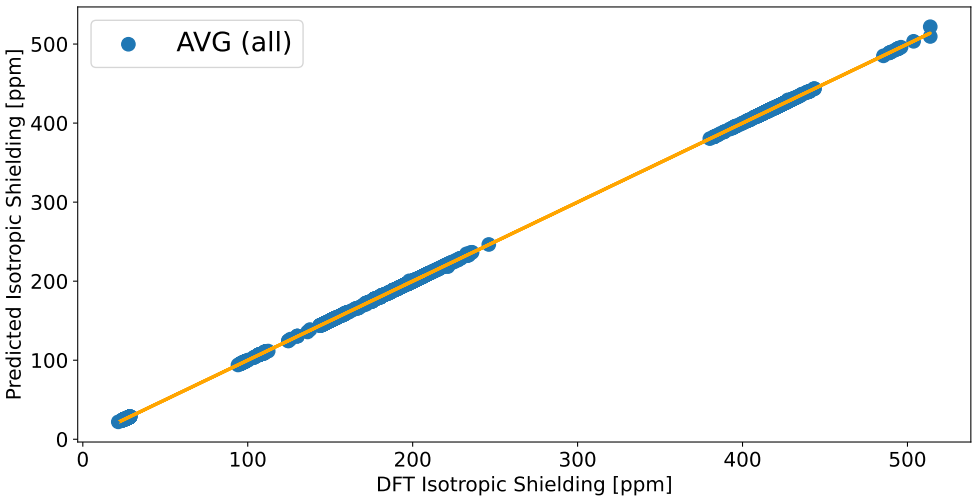

Figure S6. Predicted vs DFT isotropic shielding of all the atomic environments in the zeolites obtained with the average of the predicted ML-KRR and ML-GBR values.

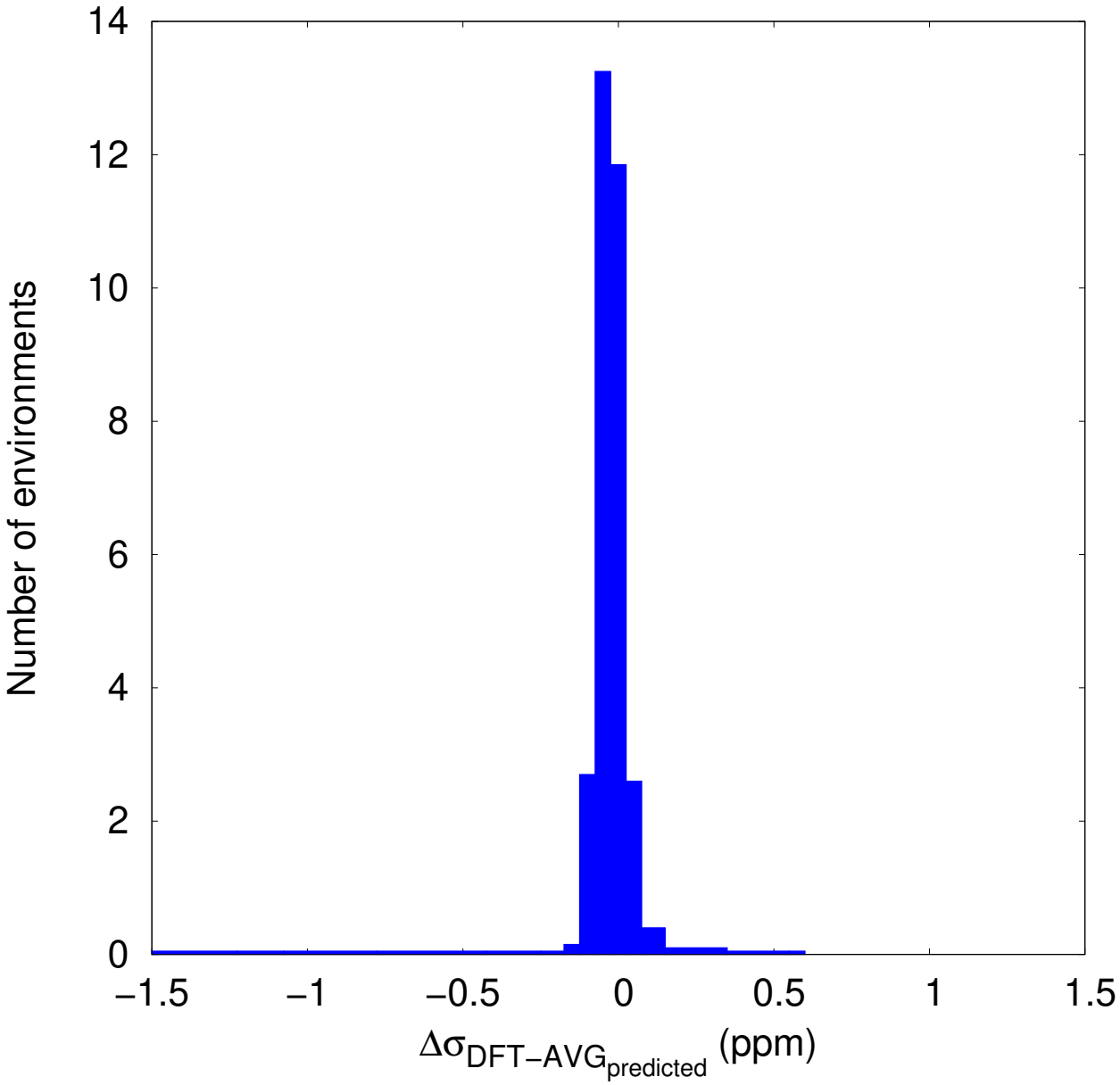

Figure S7. Distribution of the differences between the isotropic shielding values computed with DFT and the average between predicted ML-KRR and ML-GBR values. Only silicon atomic environments are considered. The histograms are obtained with an interval of 0.1 ppm in the count of the number of atomic environments.

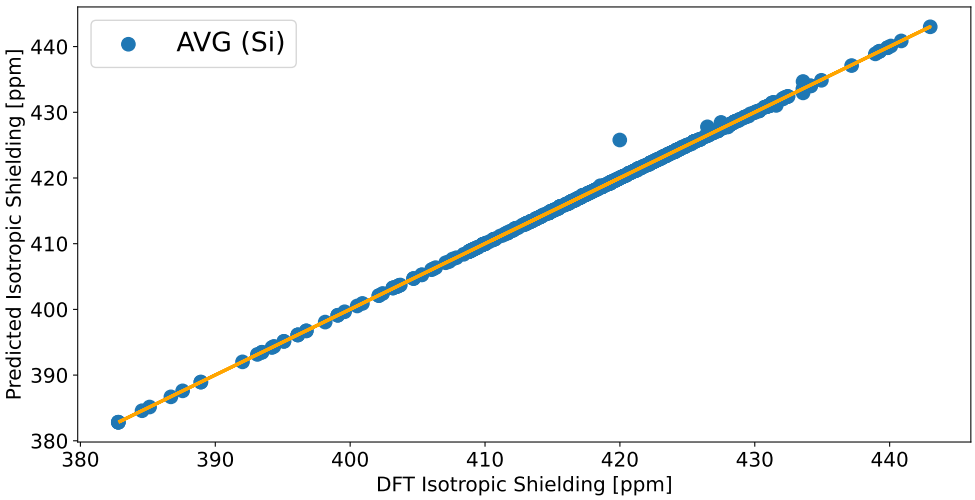

Figure S8. Predicted vs DFT isotropic shielding of silicon atomic environments in the zeolites obtained with the average of the predicted ML-KRR and ML-GBR values.

3. References

1. Baerlocher, C.; McCusker, L. Database of Zeolite Structures. http://www.iza-structure.org/databases/. Accessed: 2022-03-28.