SUPPORTING INFORMATION

Split Charge Equilibration Model and REPEAT Electrostatic Potential Fitted Charges for Periodic Frameworks with a Net Charge

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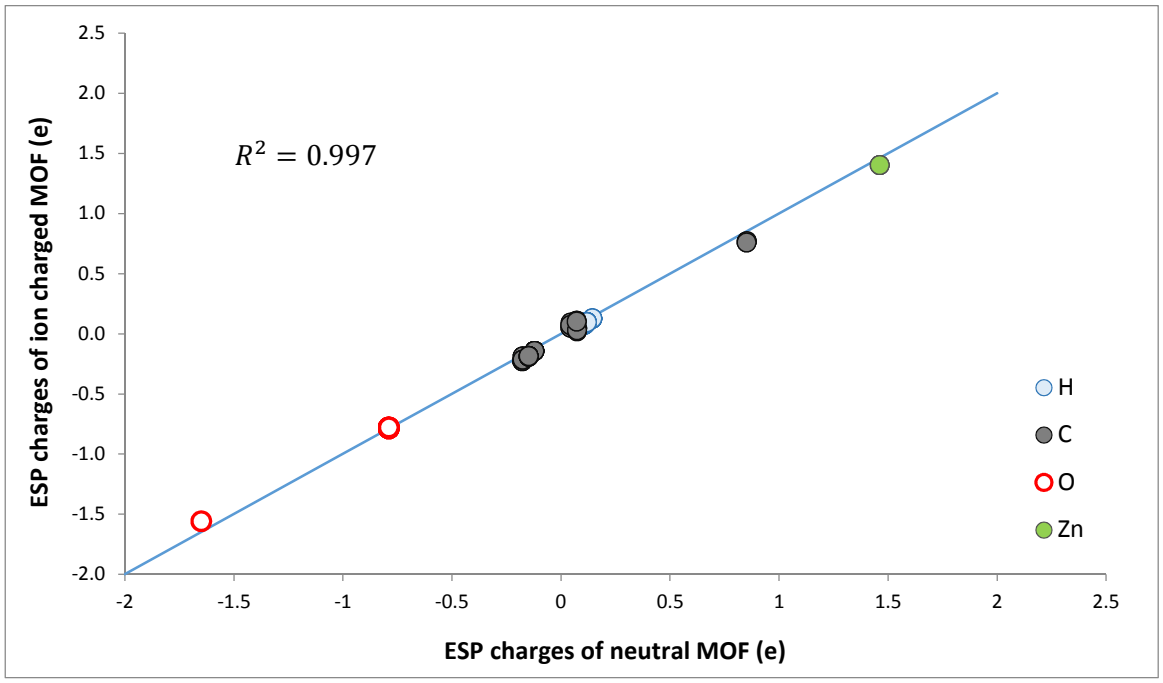

Figure S1. Comparison of ESP charges determined from periodic QM calculation of the neutral MOF IRMOF-16 to those evaluated with 2 F^- ions inserted.

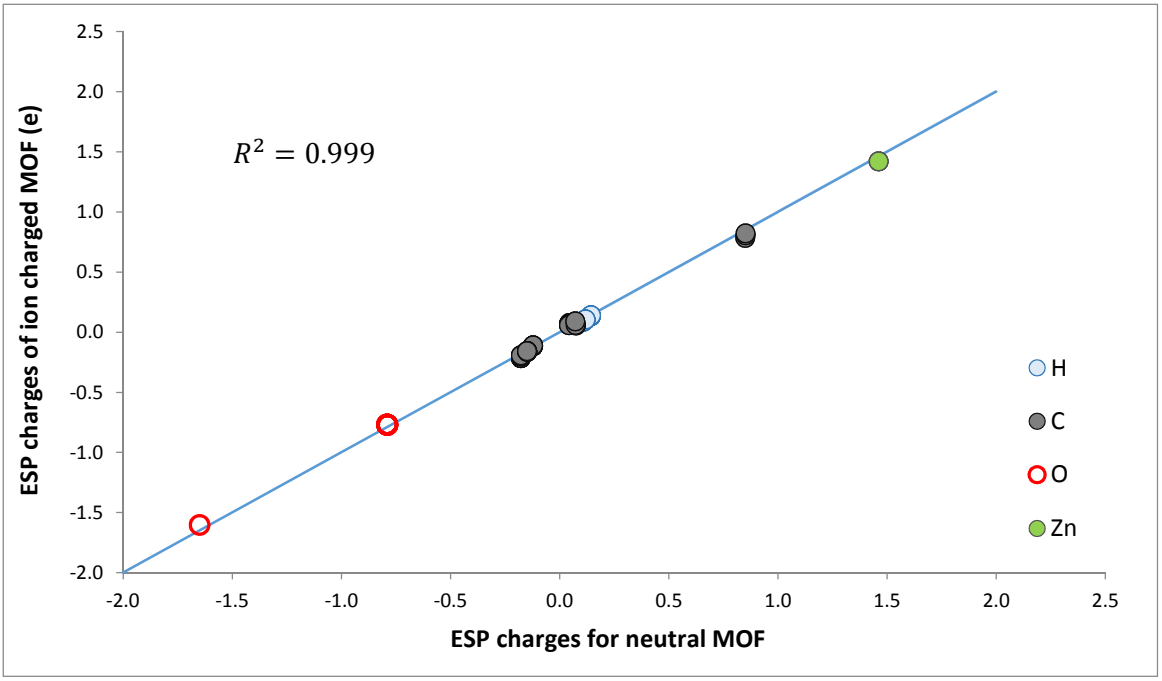

Figure S2. Comparison of ESP charges determined from periodic QM calculation of the neutral MOF IRMOF-16 to those evaluated with a F^- ion inserted.

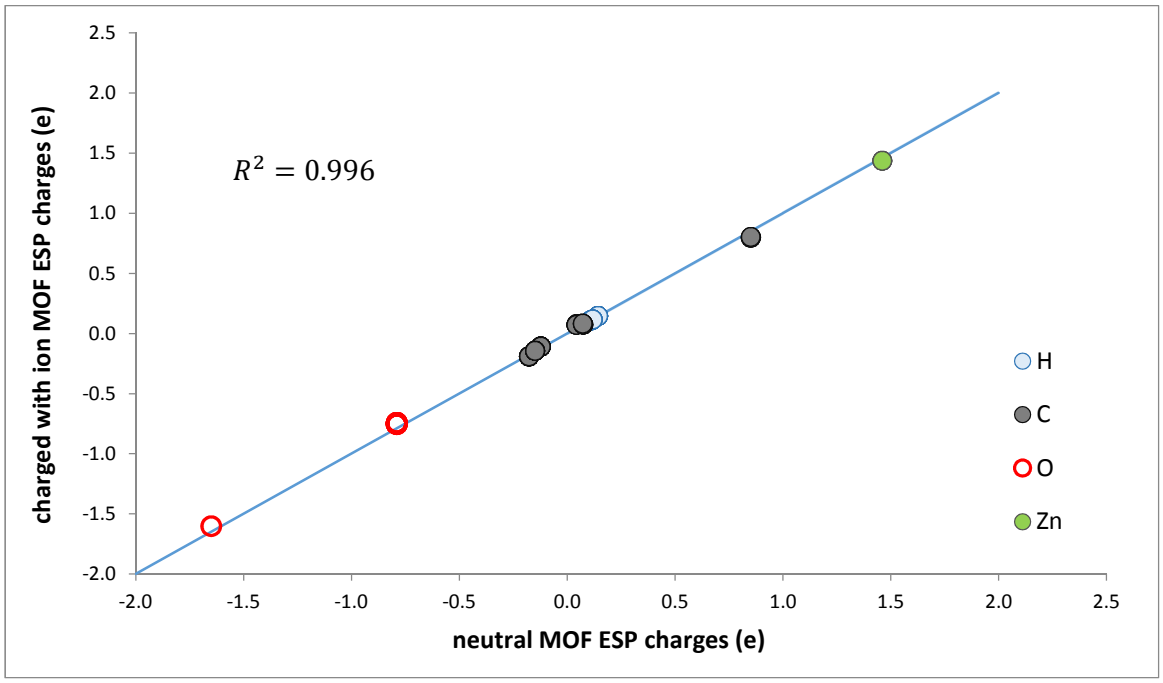

Figure S3. Comparison of ESP charges determined from periodic QM calculation of the neutral MOF IRMOF-16 to those evaluated with 2 Na^+ ions inserted.

Table S1. Difference in charges between the QEq model and REPEAT method as well as SQE_{AB} model and REPEAT method for a set of charged zeolites based on optimized parameters given in Table S2.

Base zeolite framework	Net charge of unit cell (e)	Avg. charge per atom (e)	MAD (e)	
			QEq	SQE_{AB}
ABW	-4	-0.167	0.206	0.151
FAU	-70	-0.121	0.149	0.123
LTL	-12	-0.111	0.112	0.107
EDI	-10	-0.083	0.132	0.114
LTJ	-4	-0.083	0.139	0.113
MFI	-24	-0.083	0.153	0.129
AFG	-8	-0.055	0.114	0.105
LAU	-4	-0.055	0.091	0.073
RHO	-8	-0.055	0.094	0.082
MFI	0	0.0	0.076	0.067
MRE	0	0.0	0.099	0.083
STO	0	0.0	0.082	0.070

Table S2. Optimized parameters in eV for the QEq and SQE_{AB} models based on a set of charged zeolite frameworks listed in Table S1.

Atom or bond	QEq	SQE_{AB}
κ(O)	9.9037	3.1632
κ(Al)	15.365	15.699
κ(Si)	16.163	15.238
χ(O)	6.4282	0.24229
χ(Al)	-15.582	-0.14777
χ(Si)	-11.542	0.96987
κ(O-Al)		10.1644
κ(O-Si)		10.5856
χ(O-Al)		-12.9003
χ(O-Si)		-9.8614

Brief overview of Genetic Algortihm used to fit QEq and SQE_{AB} parameters for aluminosilicate zeolites.

A custom genetic algorithm (GA) was used to fit all of the parameters simultaneously for each method separately (QEq and SQE_{AB}). The GA is initialized with the creation of multiple sets of randomly generated parameters, collectively known as a generation, that were then evaluated for how closely they reproduced the QM ESP. The new generation was formed by using a roulette wheel selection algorithm, which chooses two individuals from the generation to act as parents to new individuals by a mating algorithm. The mating algorithm selects a random value for each parameter which is between the values of each corresponding parameter for both the parents'. Subsequent mutations were allowed that would alter a given parameter by ± 30% of the parameter value. The GA was considered converged when the top performer in subsequent generations remained the same for ten generations.