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Electronic Supporting Information for "Quantifying Intuition: Bayesian Approach to Figures of Merit in EXAFS Analysis of Magic Size Clusters"

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1 Covariance Matrix Calculation

For constructing correlation matrices of results, I indexed matrices by order of parameter reported in Larch.

For example if ΔR was reported first and E0 was reported second, c_{11} of the correlation matrix would be ΔR's correlation with itself (i.e. 1), c_{12} (=c_{21}) would be the correlation between ΔR and E0.

Multiplying each element of correlation matrix by the errors of each parameter it's indexed by gives the elements of the parameter covariance matrix.

$$c_{ij} := Corr\left(X_i, X_j\right) = \frac{Cov\left(X_i, X_j\right)}{\sigma_{X_i}\sigma_{X_j}} \tag{1}$$

$(\sigma_{X_i}\sigma_{X_j} > 0)$

2 Fit Results for Ge

2.1 Model 1

Parameter correlations:

$$Corr_{model1} = \begin{pmatrix} 1 & 0.8939 & 0.0155 & 0.0952 \\ 0.8939 & 1 & 0.0016 & 0.0835 \\ 0.0155 & 0.0016 & 1 & 0.8929 \\ 0.0952 & 0.0835 & 0.8929 & 1 \end{pmatrix}$$

# FoM	Value (Ge Model 1)
χ^2	0.07853625
χ^2_μ	0.00462340
AIC	-109.27529
BIC	-105.099743
lnL	55.7087890
# FoM	Value (Ge Model 2)
χ^2	0.04449535
χ^2_μ	0.00342623
AIC	-113.199414
BIC	-104.848311
lnL	64.6744943
# FoM	Value (Ge Model 3a)
χ^2	0.68206306
χ^2_μ	0.04015282
AIC	-63.9112922
BIC	-59.7357408
LnL	85.52859223
# FoM	Value (Ge Model 3b)
χ^2	1.88762731
χ^2_μ	0.15602040
AIC	-31.5397887
BIC	-23.5345901
LnL	96.94572188

Table 1 Ge FoMs and Model.

2.2 Model 2

Parameter correlations:

$$Corr_{model2} = \begin{pmatrix} 1 & 0.7104 & 0.1260 & 0.9053 & 0.7655 & 0.1870 & -0.0173 & 0.1260 \\ 0.7104 & 1 & -0.1301 & 0.7293 & 0.4034 & 0.1620 & -0.2782 & -0.5941 \\ 0.1260 & -0.1301 & 1 & 0.1883 & 0.6647 & 0.8806 & 0.9803 & 0.8491 \\ 0.9053 & 0.7293 & 0.1883 & 1,0.6672 & 0.1720 & 0.0213 & 0.1883 & \\ 0.7655 & 0.4034 & 0.6647 & 0.6672 & 1 & 0.6969 & 0.5849 & 0.4068 \\ 0.1870 & 0.1620 & 0.8806 & 0.1720 & 0.6969 & 1 & 0.8519 & 0.6440 \\ -0.0173 & -0.2782 & 0.9803 & 0.0213 & 0.5849 & 0.8519 & 1 & 0.9192 \\ -0.2012 & -0.5941 & 0.8491 & -0.2146 & 0.4068 & 0.6440 & 0.9192 & 1 \end{pmatrix}$$

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Parameter	Value	Error
Δ R	-0.00140688	±0.00203474
E0	7.66897390	± 0.67658567
$S0^2$	0.89160567	± 0.03684971
σ^2	0.00249832	$\pm 1.7471 \times 10^{-4}$

Table 2 Ge Model 1 parameter values errors.

Parameter	Value	Error
ΔR_1	0.16479676	±0.03272449
ΔR_2	0.10219475	± 0.01338508
ΔR_3	0.00801148	± 0.01909186
E0	12.0817927	± 1.61900030
$S0^2$	0.79597733	± 0.11791880
σ_1^2	0.00626589	± 0.00402359
σ_2^2	9.7952×10^{-4}	± 0.00153078
σ_3^2	0.00108762	± 0.00118266

Table 3 Ge Model 2 parameter values and errors.

2.3 Model 3a

Resulting fit values and their errors (Model 3a):

Parameter	Value	Error
Δ R	-0.08425028	±0.00145216
E0	6.38352343	±0.48374622
$S0^2$	1.79700429	±0.05292039
σ^2	0.00258436	$\pm 1.2318 * 10^{-4}$

Table 4 Ge Model 3a parameter values and errors.

Parameter correlations were:

$$Corr_{model3a} = \begin{pmatrix} 1 & 0.89 & 0.0774 & 0.0891 \\ 0.89 & 1 & -0.0014 & 0.0128 \\ 0.0774 & 0.0014 & 1 & 0.8896 \\ 0.0891 & 0.0128 & 0.8896 & 1 \end{pmatrix}$$

2.4 Model 3b

Parameter correlations were:

$$Corr_{model3b} = \begin{pmatrix} 1 & -0.7747 & 0.2099 & 0.9023 & 0.1110 & -0.0608 & -0.1709 & 0.0988 \\ -0.7747 & 1 & -0.1111 & -0.5297 & 0.3364 & 0.5303 & -0.2704 & 0.0140 \\ 0.2099 & -0.1111 & 1 & 0.2483 & 0.0471 & 0.0027 & -0.0336 & 0.3111 \\ 0.9023 & -0.5297 & 0.2483 & 1 & 0.1340 & -0.0011 & -0.1925 & 0.0986 \\ 0.1110 & 0.3364 & 0.0471 & 0.1340 & 1 & 0.9061 & -0.6083 & 0.2088 \\ -0.0608 & 0.5303 & 0.0027 & -0.0011 & 0.9061 & 1 & -0.8166 & 0.1770 \\ -0.1709 & -0.2704 & -0.00336 & -0.1925 & -0.6083 & -0.8166 & 1 & -0.1335 \\ 0.0988 & 0.0140 & 0.3111 & 0.0986 & 0.2088 & 0.1770 & -0.1335 & 1 \end{pmatrix}$$

3 PDF Models

4 MSC Fit Results

4.1 MSC 311

Parameter	Value	Error
ΔR_1	-0.07358922	± 0.00874724
ΔR_2	-0.24820470	± 0.00507315
ΔR_3	0.17477143	± 0.06170117
E0	7.05653752	± 0.79498277
$S0^2$	1.28427500	± 0.07120701
σ_1^2	0.00425651	$\pm 8.7860 * 10^{-4}$
σ_2^2	0.00108184	$\pm 3.2113 * 10^{-4}$
σ_3^2	0.01399333	± 0.00793785

Table 5 Ge Model 3b parameters and values.

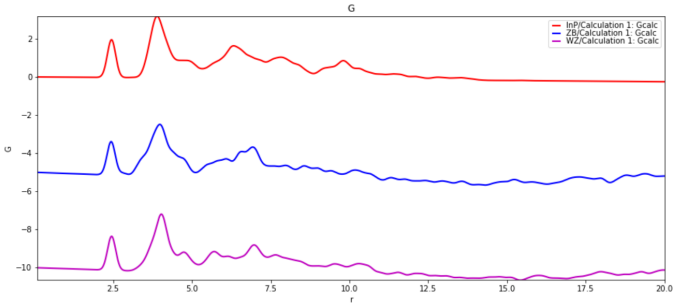

Fig. 1 Simulated xPDF spectra of 3 of the candidate models for the MSC (UFF).

# FoM	Value (zinc-blende UFF optimized)
χ^2	13.137757528397
χ^2_μ	0.80584907859888
AIC	379.685071
BIC	401.340828
# FoM	Value (β-Sn UFF optimized)
χ^2	0.95043794157651
χ^2_μ	0.95043794157651
AIC	380.597594
BIC	402.253351
# FoM	Value (InP)
χ^2	13.93767986795
χ^2_μ	0.85491503821077
AIC	391.382381
BIC	413.038138
# FoM	Value (wurtzite UFF optimized)
χ^2	29.967392960371
χ^2_μ	1.8381520554727
AIC	402.077951
BIC	423.733709

Table 6 MSC 311 UFF optimized models FoMs and values.

4.2 MSC 322

Parameter	Value	± Error
ΔR_1	0.03282165	0.06585720
ΔR_2	-0.13343322	0.05487476
ΔR_3	0.18911319	0.09005477
ΔR_4	-0.13450523	0.01369651
ΔR_5	-0.28647788	0.10385472
ΔR_6	-0.02413652	0.00697081
E0	5.87220860	1.20700151
$S0^2$	1.49999995	0.17847886
σ_1^2	0.00918721	0.00679341
σ_2^2	0.00852422	0.00548349
σ_3^2	0.01452069	0.01101530
σ_4^2	0.00231760	0.00158804
σ_5^2	0.00830576	0.01416707
σ_6^2	0.00161413	7.58707e-4
Cd-O 3rd Cumulant	-0.01941486	0.00586668

Table 10 InP MSC 311 parameter results from fit.

Parameter	Value	± Error
ΔR_1	-0.36208142	0.23963249
ΔR_2	0.07287854	0.14333625
ΔR_3	0.50762678	0.34932255
ΔR_4	-0.24955348	0.35414932
ΔR_5	0.21182778	0.10401378
ΔR_6	0.07725703	0.02016184
E0	7.08420397	2.34319246
$S0^2$	1.42978990	0.50228890
σ_1^2	0.02915404	0.03711877
σ_2^2	0.01330498	0.01405962
σ_3^2	0.02243392	0.05272623
σ_4^2	0.02615848	0.08296747
σ_5^2	2.4237e-11	0.05548291
σ_6^2	4.28522e-4	0.00548038
Cd-O 3rd Cumulant	-5.21710e-4	9.83225e-4

Table 11 UFF Optimized wurtzite MSC 311 parameter results from fit.

Parameter	Value	± Error
ΔR_1	-0.34994115	0.13702574
ΔR_2	-0.06768343	0.32504253
ΔR_3	-0.17602182	0.07240709
ΔR_4	0.11949714	0.07272283
ΔR_5	0.04062348	0.01474340
ΔR_6	-0.04456645	0.00963823
E0	2.84276927	1.08080816
$S0^2$	0.76047743	0.08128971
σ_1^2	0.01916003	0.01866999
σ_2^2	0.02532326	0.05172049
σ_3^2	0.01006357	0.00728044
σ_4^2	0.01050630	0.00603681
σ_5^2	2.55050e-4	0.00125294
σ_6^2	0.00406757	0.00165866
Cd-O 3rd Cumulant	0.01214339	0.00209641

Table 12 DFT Optimized Zinc-Blende MSC 311 parameter results from fit.

Parameter	Value	± Error
ΔR_1	0.21697410	0.09682118
ΔR_2	-0.06512601	0.06428268
ΔR_3	0.22007272	0.05145213
ΔR_4	-0.31934560	0.07807775
ΔR_5	0.54021927	0.14498515
ΔR_6	0.13342227	0.01390976
E0	8.14020385	2.50377827
$S0^2$	1.50000000	8.68691925
σ_1^2	0.01380318	0.01252344
σ_2^2	0.01158087	0.00767517
σ_3^2	2.91419e-8	0.11364470
σ_4^2	0.06666964	0.01949219
σ_5^2	0.03285543	0.03358842
σ_6^2	8.02916e-4	0.00392128
Cd-O 3rd Cumulant	-6.20498e-4	3.57972e-4

Table 13 DFT Optimized β-Sn MSC 311 parameter results from fit.

Parameter	Value	± Error
ΔR_1	0.02141792	0.18161926
ΔR_2	-0.00165774	0.07476340
ΔR_3	-0.43781025	0.20347274
ΔR_4	-0.45685489	0.08612126
ΔR_5	-0.02671040	0.01212220
ΔR_6	0.05492013	0.01026264
E0	4.05417799	1.60404493
$S0^2$	1.49999993	0.11845651
σ_1^2	0.03146840	0.03024400
σ_2^2	0.01339112	0.00880531
σ_3^2	0.02538696	0.04047429
σ_4^2	0.04556082	0.00988582
σ_5^2	0.00220769	0.00204737
σ_6^2	0.00105537	0.00157574
Cd-O 3rd Cumulant	-0.01996019	0.01152446

Table 14 DFT Optimized wurtzite MSC 311 parameter results from fit.

# FoM	Value (zinc-blende UFF optimized)
χ^2	15.926460990271
χ^2_μ	1.3300869375539
AIC	316.167274
BIC	335.590424
# FoM	Value (β-Sn UFF optimized)
χ^2	15.307879335878
χ^2_μ	1.2784265354834
AIC	312.148308
BIC	331.571458
# FoM	Value (InP)
χ^2	16.2250748348
χ^2_μ	1.3550254580591
AIC	311.527681
BIC	330.950831
# FoM	Value (wurtzite UFF optimized)
χ^2	30.859903297829
χ^2_μ	2.5772426338591
AIC	329.687977
BIC	349.111127

Table 15 MSC 322 UFF optimized models FoMs and values.

Parameter	Value	± Error
ΔR_1	0.26137530	0.16775917
ΔR_2	-0.17593065	0.04296148
ΔR_3	-0.06312106	0.06681595
ΔR_4	0.25080242	0.08385056
ΔR_5	-0.02224874	0.01211012
ΔR_6	-0.16729583	0.01387111
E0	0.09173737	1.48742868
$S0^2$	1.40568587	0.21924580
σ_1^2	0.01718823	0.02603750
σ_2^2	0.00679538	0.00472036
σ_3^2	0.00779194	0.00732691
σ_4^2	0.01652390	0.00780238
σ_5^2	2.8183e-12	0.00136431
σ_6^2	0.00125238	0.00230185
Cd-O 3rd Cumulant	0.01231496	0.00333574

Table 19 InP MSC 322 parameter results from fit.

Parameter	Value	± Error
ΔR_1	0.12798502	0.07550860
ΔR_2	0.19276246	0.14065870
ΔR_3	0.29993629	0.20369988
ΔR_4	0.43416447	0.22987701
ΔR_5	0.19146239	0.14543783
ΔR_6	0.05588295	0.02300390
E0	5.17380861	3.36479509
$S0^2$	1.38137412	0.58754007
σ_1^2	0.00606287	0.00636685
σ_2^2	0.00717252	0.01145102
σ_3^2	0.01106489	0.02431202
σ_4^2	0.01353443	0.02885406
σ_5^2	2.2545e-10	0.02020385
σ_6^2	1.42868e-4	0.00647707
Cd-O 3rd Cumulant	-4.28971e-4	0.00166953

Table 20 UFF Optimized wurtzite MSC 322 parameter results from fit.

Parameter	Value	± Error
ΔR_1	0.36252966	0.07083651
ΔR_2	0.15025876	0.05150959
ΔR_3	0.30511885	0.22963269
ΔR_4	-0.07138511	0.16908217
ΔR_5	-0.13002954	0.02247162
ΔR_6	-0.00833200	0.01334105
E0	1.53702247	1.61381336
$S0^2$	0.67968552	0.20150179
σ_1^2	0.00347392	0.00803017
σ_2^2	0.00271259	0.00564498
σ_3^2	0.01204499	0.02686456
σ_4^2	0.00689435	0.00982757
σ_5^2	1.5590e-11	0.28406968
σ_6^2	0.00135599	0.00284600
Cd-O 3rd Cumulant	0.00239180	0.00318068

Table 21 DFT Optimized Zinc-Blende MSC 322 parameter results from fit.

Parameter	Value	± Error
ΔR_1	0.04143835	0.04388104
ΔR_2	0.38297088	0.14661145
ΔR_3	0.45670560	0.07737136
ΔR_4	-0.52892596	0.09638376
ΔR_5	0.11306472	0.01080273
ΔR_6	-0.22183722	0.01238124
E0	0.21052467	1.39568464
$S0^2$	1.45555711	0.20491087
σ_1^2	0.01088980	0.00476725
σ_2^2	0.01780873	0.02049128
σ_3^2	0.01692651	0.00712260
σ_4^2	0.01796559	0.01847393
σ_5^2	2.8765e-12	9.04096e-4
σ_6^2	0.00131603	0.00199730
Cd-O 3rd Cumulant	0.01186675	0.00304264

Table 22 DFT Optimized β-Sn MSC 322 parameter results from fit.

Parameter	Value	± Error
ΔR_1	0.11484025	0.05265343
ΔR_2	-0.18173499	0.06074060
ΔR_3	-0.15420714	0.04215927
ΔR_4	-0.58619141	0.09774641
ΔR_5	0.06046623	0.01270421
ΔR_6	-0.07166987	0.01444723
E0	2.11658729	2.02049453
$S0^2$	1.49999997	0.10647122
σ_1^2	0.00969107	0.00522226
σ_2^2	0.01522373	0.00791888
σ_3^2	0.00833431	0.00391406
σ_4^2	0.05075435	0.01298503
σ_5^2	5.7362e-12	7.72006e-4
σ_6^2	0.00105040	0.00213648
Cd-O 3rd Cumulant	-0.03277052	0.01242642

Table 23 DFT Optimized wurtzite MSC 322 parameter results from fit.