

Supplementary Information for “An Optimized Charge Penetration Model for Use with the AMOEBA Force Field” by Rackers, Wang, Liu, Piquemal, Ren and Ponder

1. Damping Functions for Higher-order Damping

(Functions given in the same form as eq. 5 of Ref. 1)

A. One-site damping functions

$$\lambda_1 = 1 - e^{-\alpha r}$$

$$\lambda_3 = 1 - (1 + \alpha r)e^{-\alpha r}$$

$$\lambda_5 = 1 - \left(1 + \alpha r + \left(\frac{1}{3}\right)(\alpha r)^2\right)e^{-\alpha r}$$

B. Two site damping functions, $\alpha_i \neq \alpha_k$

$$A = \frac{\alpha_k^2}{\alpha_k^2 - \alpha_i^2}, \quad B = \frac{\alpha_i^2}{\alpha_i^2 - \alpha_k^2}$$

$$\lambda_1 = 1 - Ae^{-\alpha_i r} - Be^{-\alpha_k r}$$

$$\lambda_3 = 1 - (1 + \alpha_i r)Ae^{-\alpha_i r} - (1 + \alpha_k r)Be^{-\alpha_k r}$$

$$\lambda_5 = 1 - \left(1 + \alpha_i r + \left(\frac{1}{3}\right)(\alpha_i r)^2\right)Ae^{-\alpha_i r} - \left(1 + \alpha_k r + \left(\frac{1}{3}\right)(\alpha_k r)^2\right)Be^{-\alpha_k r}$$

$$\lambda_7 = 1 - \left(1 + \alpha_i r + \left(\frac{2}{5}\right)(\alpha_i r)^2 + \left(\frac{1}{15}\right)(\alpha_i r)^3\right)Ae^{-\alpha_i r} \\ - \left(1 + \alpha_k r + \left(\frac{2}{5}\right)(\alpha_k r)^2 + \left(\frac{1}{15}\right)(\alpha_k r)^3\right)Be^{-\alpha_k r}$$

$$\lambda_9 = 1 - \left(1 + \alpha_i r + \left(\frac{3}{7}\right)(\alpha_i r)^2 + \left(\frac{2}{21}\right)(\alpha_i r)^3 + \left(\frac{1}{105}\right)(\alpha_i r)^4\right)Ae^{-\alpha_i r} \\ - \left(1 + \alpha_k r + \left(\frac{3}{7}\right)(\alpha_k r)^2 + \left(\frac{2}{21}\right)(\alpha_k r)^3 + \left(\frac{1}{105}\right)(\alpha_k r)^4\right)Be^{-\alpha_k r}$$

C. Two site damping functions, $\alpha_i = \alpha_k$

$$\lambda_1 = 1 - \left(1 + \left(\frac{1}{2}\right)\alpha r\right)e^{-\alpha r}$$

$$\lambda_3 = 1 - \left(1 + ar + \left(\frac{1}{2}\right)(\alpha_i r)^2\right) e^{-ar}$$

$$\lambda_5 = 1 - \left(1 + ar + \left(\frac{1}{2}\right)(\alpha_i r)^2 + \left(\frac{1}{6}\right)(\alpha_i r)^3\right) e^{-ar}$$

$$\lambda_7 = 1 - \left(1 + ar + \left(\frac{1}{2}\right)(\alpha_i r)^2 + \left(\frac{1}{6}\right)(\alpha_i r)^3 + \left(\frac{1}{30}\right)(\alpha_i r)^4\right) e^{-ar}$$

$$\lambda_9 = 1 - \left(1 + ar + \left(\frac{1}{2}\right)(\alpha_i r)^2 + \left(\frac{1}{6}\right)(\alpha_i r)^3 + \left(\frac{4}{105}\right)(\alpha_i r)^4 + \left(\frac{1}{210}\right)(\alpha_i r)^5\right) e^{-ar}$$

2. S101x7 SAPT Electrostatics Fit Statistics

Multipole Only		
RMSE (Root Mean Square Error)	0.7 – 0.8	24.16611265
	0.9 – 1.1	4.350677453
	Total	13.43047692
MSE (Mean Signed Error)	0.7 – 0.8	19.15611117
	0.9 – 1.1	3.160407234
	Total	7.730608359
MUE (Mean Unsigned Error)	0.7 – 0.8	19.15611117
	0.9 – 1.1	3.160407234
	Total	7.730608359
Mean Percent Error	0.7 – 0.8	0.692902042
	0.9 – 1.1	1.330447394
	Total	57.41457894
Mean Absolute Percent Error	0.7 – 0.8	0.692902042
	0.9 – 1.1	1.330447394
	Total	57.41457894

Model 1 – Charge-charge – Element-based Parameters		
RMSE (Root Mean Square Error)	0.7 – 0.8	3.530462178
	0.9 – 1.1	1.079421339
	Total	2.096053384
MSE (Mean Signed Error)	0.7 – 0.8	0.070609574
	0.9 – 1.1	0.443082553
	Total	0.336661702
MUE (Mean Unsigned Error)	0.7 – 0.8	2.483826596
	0.9 – 1.1	0.699765532

	Total	1.209497264
Mean Percent Error	0.7 – 0.8	0.014649782
	0.9 – 1.1	0.083136474
	Total	3.178442377
Mean Absolute Percent Error	0.7 – 0.8	0.100161271
	0.9 – 1.1	0.247685764
	Total	10.27679545

Model 2 – Charge-charge – Element-based Parameters		
RMSE (Root Mean Square Error)	0.7 – 0.8	3.416100288
	0.9 – 1.1	1.196352255
	Total	2.087232479
MSE (Mean Signed Error)	0.7 – 0.8	0.078644681
	0.9 – 1.1	-0.51620766
	Total	-0.346249848
MUE (Mean Unsigned Error)	0.7 – 0.8	2.524932979
	0.9 – 1.1	0.885186383
	Total	1.35368541
Mean Percent Error	0.7 – 0.8	-0.024265813
	0.9 – 1.1	-0.456742535
	Total	-16.65888785
Mean Absolute Percent Error	0.7 – 0.8	0.110418585
	0.9 – 1.1	0.537220758
	Total	20.76386398

Model 3 – Charge-charge – Element-based Parameters		
RMSE (Root Mean Square Error)	0.7 – 0.8	8.245733619
	0.9 – 1.1	1.070226765
	Total	4.499383648
MSE (Mean Signed Error)	0.7 – 0.8	0.988135106
	0.9 – 1.1	0.034202979
	Total	0.306755015
MUE (Mean Unsigned Error)	0.7 – 0.8	3.662237234
	0.9 – 1.1	0.671327234
	Total	1.525872948
Mean Percent Error	0.7 – 0.8	0.036913509
	0.9 – 1.1	0.046321109
	Total	2.181661167
Mean Absolute Percent Error	0.7 – 0.8	0.166713556
	0.9 – 1.1	0.39171247
	Total	16.37135331

Model 1 – Charge-charge – Class-based Parameters		
RMSE (Root Mean Square Error)	0.7 – 0.8	2.746166031
	0.9 – 1.1	0.989597309
	Total	1.689436504
MSE (Mean Signed Error)	0.7 – 0.8	0.087677128
	0.9 – 1.1	0.396219574
	Total	0.30806459
MUE (Mean Unsigned Error)	0.7 – 0.8	1.970433511
	0.9 – 1.1	0.633159574
	Total	1.015237842
Mean Percent Error	0.7 – 0.8	0.00351084
	0.9 – 1.1	0.034173836
	Total	1.270649006
Mean Absolute Percent Error	0.7 – 0.8	0.081690656
	0.9 – 1.1	0.225204723
	Total	9.210035191

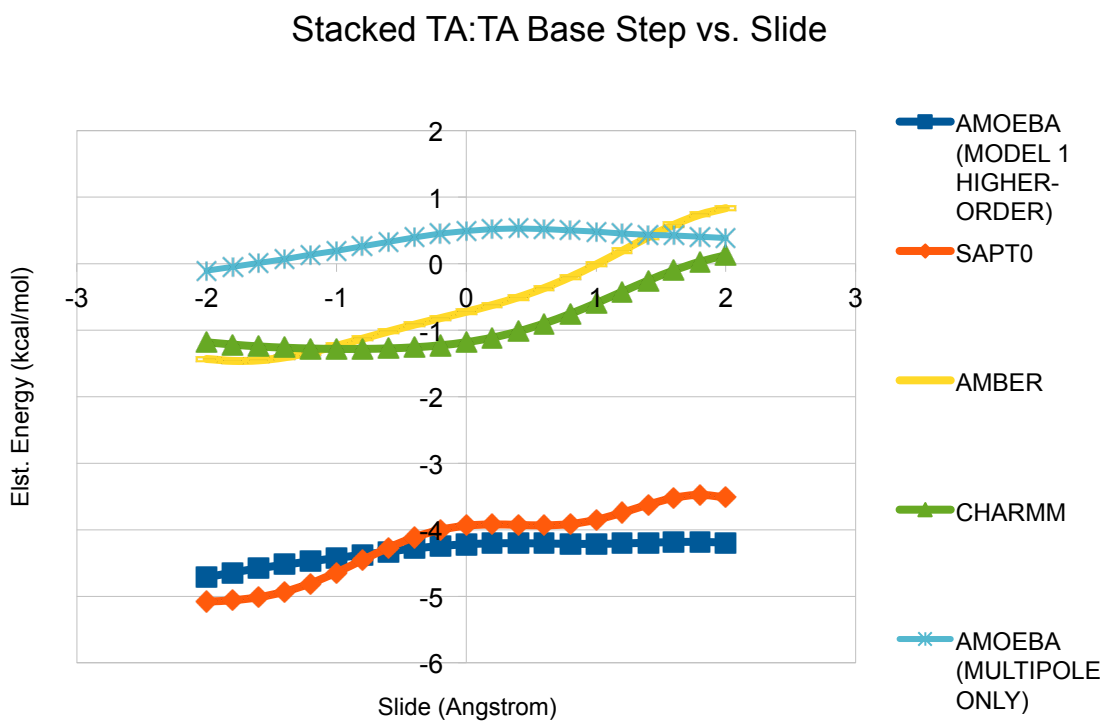
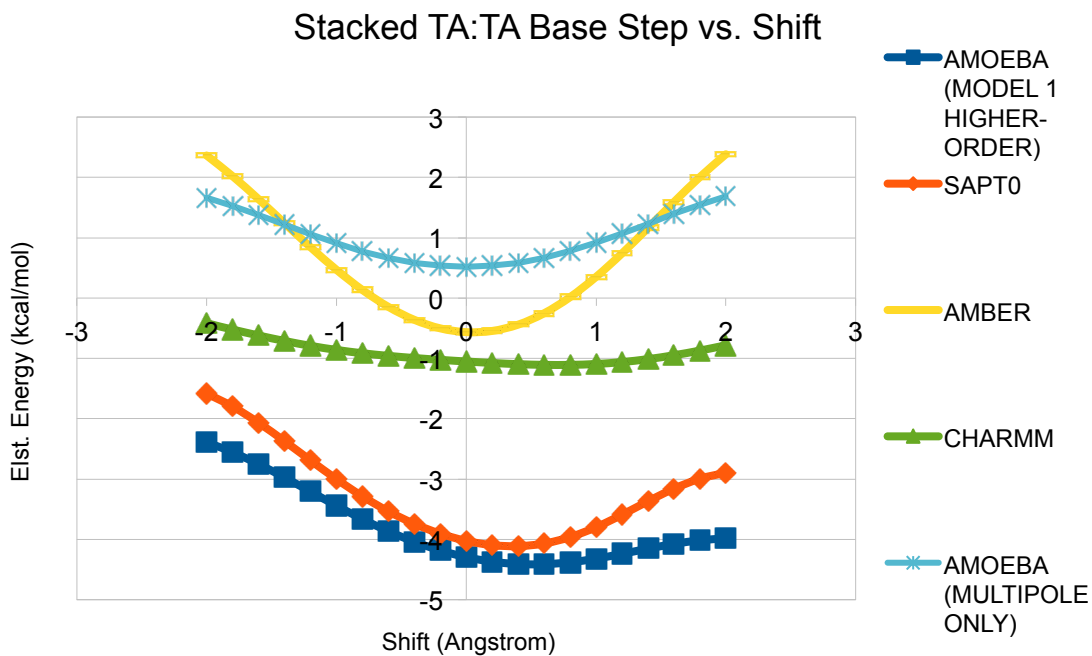
Model 2 – Charge-charge – Class-based Parameters		
RMSE (Root Mean Square Error)	0.7 – 0.8	3.038892269
	0.9 – 1.1	1.043989404
	Total	1.848524579
MSE (Mean Signed Error)	0.7 – 0.8	0.03548617
	0.9 – 1.1	-0.415489574
	Total	-0.286639362
MUE (Mean Unsigned Error)	0.7 – 0.8	2.32576383
	0.9 – 1.1	0.759034255
	Total	1.206671277
Mean Percent Error	0.7 – 0.8	-0.024980534
	0.9 – 1.1	-0.379144054
	Total	-13.89772384
Mean Absolute Percent Error	0.7 – 0.8	0.104954218
	0.9 – 1.1	0.463356585
	Total	18.04779542

Model 1 – Higher-order – Class-based Parameters		
RMSE (Root Mean Square Error)	0.7 – 0.8	2.274214573
	0.9 – 1.1	0.566506743
	Total	1.306508613
MSE (Mean Signed Error)	0.7 – 0.8	0.047035638
	0.9 – 1.1	0.013938085

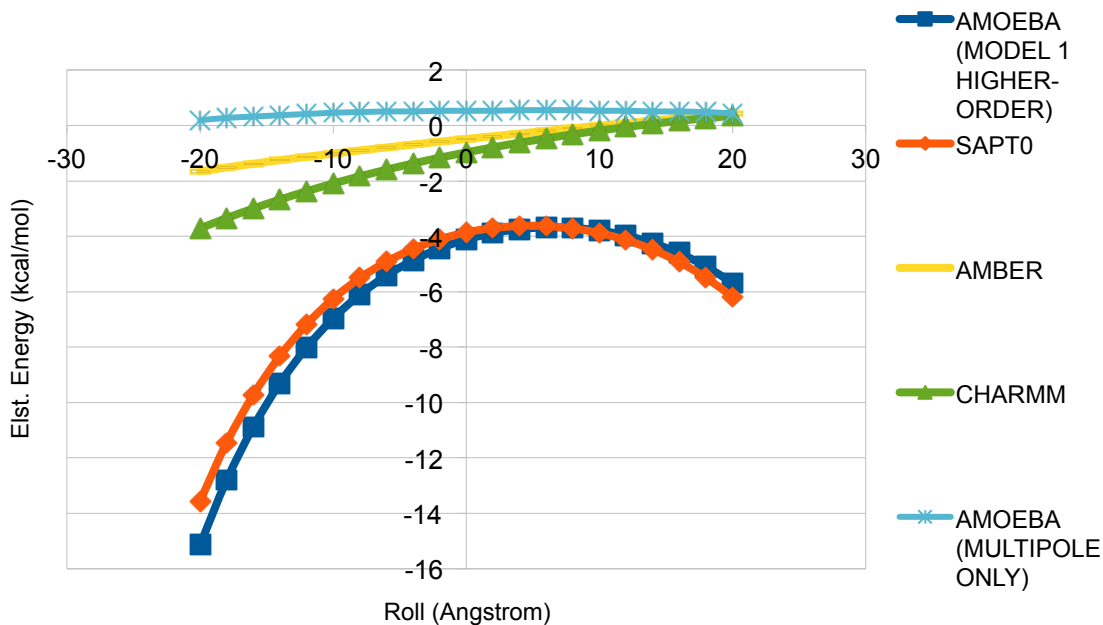
	Total	0.023394529
MUE (Mean Unsigned Error)	0.7 – 0.8	1.529532447
	0.9 – 1.1	0.376271277
	Total	0.705774468
Mean Percent Error	0.7 – 0.8	-0.003770317
	0.9 – 1.1	-0.044059741
	Total	-1.627423843
Mean Absolute Percent Error	0.7 – 0.8	0.061419216
	0.9 – 1.1	0.18531193
	Total	7.495700609

Model 2 – Higher-order – Class-based Parameters		
RMSE (Root Mean Square Error)	0.7 – 0.8	2.639920385
	0.9 – 1.1	0.661324567
	Total	1.517757283
MSE (Mean Signed Error)	0.7 – 0.8	0.009317553
	0.9 – 1.1	-0.115076596
	Total	-0.07953541
MUE (Mean Unsigned Error)	0.7 – 0.8	1.817476064
	0.9 – 1.1	0.466214043
	Total	0.852288906
Mean Percent Error	0.7 – 0.8	-0.013435382
	0.9 – 1.1	-0.151155074
	Total	-5.590329517
Mean Absolute Percent Error	0.7 – 0.8	0.074795428
	0.9 – 1.1	0.248929303
	Total	9.958838368

3. TA:TA Step Plots for Nucleic Acid Base Structural Parameters



Stacked TA:TA Base Step vs. Roll



Stacked TA:TA Base Step vs. Twist

