$RMSE(E_{int}^{\mathit{EMLE}}, E_{int}^{\mathit{QM/MM}})$	$RMSE(E_{static}^{\mathit{EMLE}}, E_{static}^{\mathit{QM/MM}})$	$RMSE(E_{ind}^{EMLE}, E_{ind}^{QM/MM})$
2.18 2.19 1.34 1.37 1.32 1.37 0.99 0.96 1.03 0.99	2.21 2.21 1.42 1.42 1.40 1.40 0.94 0.94 0.97 0.97	0.50 0.42 0.38 0.30 0.38 0.29 0.28 0.19 0.30 0.20 -2.0 10 10 10 10 10 10 10 10 10 10 10 10 10
2.52 2.52 1.60 1.62 1.58 1.61 1.17 1.13 1.09 1.03	2.56 2.56 1.63 1.63 1.60 1.60 1.05 1.05 1.01 1.01	0.72 0.63 0.43 0.33 0.43 0.32 0.36 0.27 0.33 0.21  -1.5   S   S   S   S   S   S   S   S   S
2.52 2.52 1.60 1.62 1.58 1.61 1.17 1.13 1.09 1.03 2.51 2.52 1.51 1.54 1.53 1.58 1.07 1.03 1.02 1.01	2.53 2.53 1.58 1.58 1.60 1.60 0.99 0.99 0.98 0.98	0.68 0.58 0.42 0.32 0.42 0.32 0.34 0.24 0.32 0.21 $^{-1.0}$ $\stackrel{\square}{\mathbb{Z}}$
$MSE(E_{int}^{\mathit{EMLE}}, E_{int}^{\mathit{QM/MM}})$	$MSE(E^{\mathit{EMLE}}_{\mathit{static}}, E^{\mathit{QM/MM}}_{\mathit{static}})$	$MSE(E_{ind}^{EMLE}, E_{ind}^{QM/MM})$
-0.02 -0.07 -0.34 -0.43 -0.33 -0.43 -0.03 -0.06 0.17 0.12	-0.14 -0.14 -0.55 -0.55 -0.54 -0.54 -0.10 -0.10 0.03 0.03	0.110.070.210.120.210.110.060.040.140.10
Testing Dataset  -0.02 -0.07 -0.34 -0.43 -0.33 -0.43 -0.03 -0.06 0.17 0.12  -0.15 -0.17 -0.59 -0.66 -0.56 -0.66 -0.34 -0.36 -0.01 -0.04  -0.19 -0.21 -0.59 -0.67 -0.64 -0.74 -0.28 -0.30 -0.12 -0.16	-0.10 -0.10 -0.75 -0.75 -0.72 -0.72 -0.30 -0.30 -0.08 -0.08	-0.05-0.080.16 0.09 0.16 0.07-0.04-0.060.08 0.04 0.2 \frac{\xi}{10} 0.4 \frac{\xi}{2}
-0.19 -0.21 -0.59 -0.67 -0.64 -0.74 -0.28 -0.30 -0.12 -0.16	-0.18 -0.18 -0.77 -0.77 -0.81 -0.81 -0.26 -0.26 -0.20 -0.20	-0.01-0.030.18 0.10 0.17 0.08-0.02-0.040.09 0.050.8
$MUE(E_{int}^{\mathit{EMLE}}, E_{int}^{\mathit{QM/MM}})$	$MUE(E_{static}^{\mathit{EMLE}}, E_{static}^{\mathit{QM/MM}})$	$MUE(E_{ind}^{\mathit{EMLE}}, E_{ind}^{\mathit{QM/MM}})$
1.59 1.60 1.01 1.06 1.01 1.06 0.75 0.73 0.78 0.75	1.60 1.60 1.10 1.10 1.09 1.09 0.72 0.72 0.74 0.74	0.37 0.31 0.28 0.22 0.28 0.21 0.20 0.13 0.22 0.15
1.82 1.79 1.19 1.23 1.16 1.22 0.87 0.84 0.82 0.79	1.77 1.77 1.24 1.24 1.22 1.22 0.80 0.80 0.77 0.77	0.51 0.43 0.32 0.23 0.32 0.23 0.25 0.18 0.24 0.15 - 1.0 g
1.82 1.79 1.19 1.23 1.16 1.22 0.87 0.84 0.82 0.79 1.83 1.82 1.13 1.18 1.14 1.21 0.82 0.79 0.78 0.76	1.78 1.78 1.21 1.21 1.23 1.23 0.76 0.76 0.75 0.75	0.51 0.43 0.32 0.23 0.32 0.23 0.25 0.18 0.24 0.15 -1.0 $\frac{1}{10}$ 0.48 0.40 0.31 0.23 0.31 0.23 0.24 0.17 0.23 0.15 -0.5 $\frac{1}{10}$
$R^2(E_{int}^{EMLE},E_{int}^{QM/MM})$	$R^2(E_{static}^{EMLE},E_{static}^{QM/MM})$	$R^{2}(E_{ind}^{EMLE}, E_{ind}^{QM/MM})$
0.94 0.94 0.98 0.98 0.98 0.99 0.99 0.99 0.99 0.99	0.92 0.92 0.97 0.97 0.97 0.99 0.99 0.98 0.98	0.91 0.94 0.95 0.97 0.95 0.97 0.99 0.97 0.99 -0.98
O.95 O.95 O.98 O.98 O.98 O.99 O.99 O.99 O.99 O.99	0.93 0.93 0.97 0.97 0.97 0.99 0.99 0.99 0.99	$0.89\ 0.92\ 0.96\ 0.98\ 0.96\ 0.98\ 0.97\ 0.98\ 0.98\ 0.99$
Testing D    1	0.93 0.93 0.97 0.97 0.97 0.99 0.99 0.99 0.99	0.90 0.93 0.96 0.98 0.96 0.98 0.97 0.99 0.98 0.99 - 0.90
$ ho(E_{int}^{\it EMLE},E_{int}^{\it QM/MM})$	$ ho(E_{static}^{EMLE}, E_{static}^{QM/MM})$	$ ho(E_{ind}^{EMLE}, E_{ind}^{QM/MM})$
0.97 0.97 0.99 0.99 0.99 0.99 0.99 0.99	0.96 0.96 0.99 0.99 0.99 0.99 0.99 0.99	0.96 0.97 0.98 0.99 0.99 0.99 0.99 0.99 0.99 - 0.99
ling Datas liter2   Iter2	0.97 0.97 0.99 0.99 0.99 0.99 0.99 0.99	0.96 0.97 0.98 0.99 0.99 0.99 0.99 0.99 1.00
Testing 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.0	0.97 0.97 0.99 0.99 0.99 0.99 0.99 0.99	0.96 0.97 0.98 0.99 0.98 0.99 0.99 1.00 0.99 1.00
$ au(E_{int}^{\it EMLE},E_{int}^{\it QM/MM})$	-(⊏EMLE ⊏QM/MM)	$\tau(E_{ind}^{EMLE}, E_{ind}^{QM/MM})$
1 (E <sub>int</sub> -, E <sub>int</sub> )  0.87 0.87 0.91 0.91 0.91 0.93 0.93 0.93 0.93	$ au(E_{static}^{EMLE}, E_{static}^{QM/MM})$ 0.85 0.85 0.90 0.90 0.90 0.90 0.92 0.92 0.92 0.92	0.82 0.86 0.89 0.91 0.89 0.91 0.94 0.91 0.94
Oata 0.88 0.88 0.93 0.92 0.94 0.94 0.94 0.94 0.94	0.86 0.86 0.91 0.91 0.91 0.93 0.93 0.93 0.93	0.84 0.87 0.90 0.92 0.90 0.92 0.94 0.92 0.94
asting a lite		-0.90
0.88 0.88 0.93 0.93 0.93 0.94 0.94 0.94 0.94	0.86 0.86 0.91 0.91 0.91 0.91 0.93 0.93 0.93	0.84 0.87 0.91 0.92 0.91 0.92 0.92 0.94 0.92 0.94 - 0.85
-Species eference ies-Iter1 ies-Iter1 ies-Iter2	-Species eference ies-Iter1 ies-Iter1 ies-Iter2	-Species eference ies-Iter1 ies-Iter1 ies-Iter2 ies-Iter2
QM7-Re QM7-Re Referen Referen Referen Referen	QM7-Species Bespoke-Species-Iter Spoke-Reference-Iter Spoke-Reference-Iter Spoke-Reference-Iter tched-Reference-Iter tched-Reference-Iter tched-Reference-Iter tched-Reference-Iter	QM7-Re QM7-Re Referen Referen Referen Referen Referen
QM' Bespoke-Sefe Bespoke-Refe Patched-Seter Patched-Sefe	QM7-Specie Bespoke-Species-Iter Bespoke-Reference-Iter Bespoke-Reference-Iter Patched-Species-Iter Patched-Reference-Iter	QM7, Bespoke-Sp Bespoke-Refer Bespoke-Refer Patched-Refer Patched-Refer
m m m m m m m m m m m m m m m m m m m	<u> </u>	ă ă ă