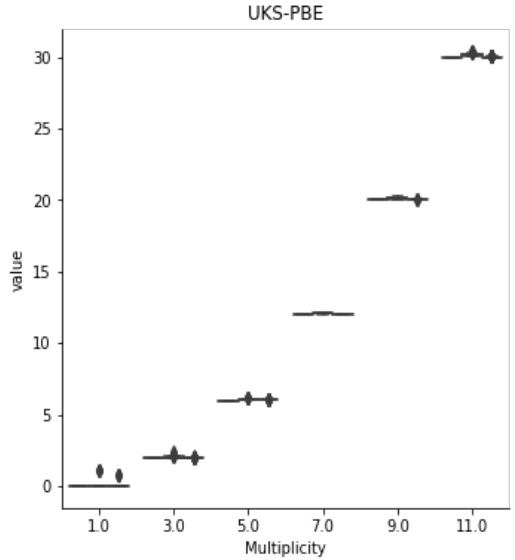
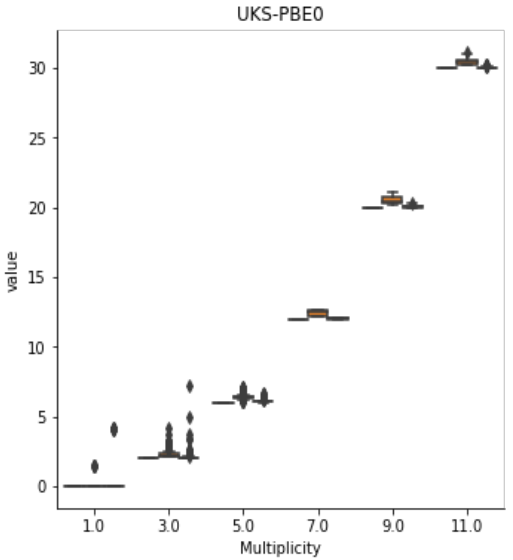
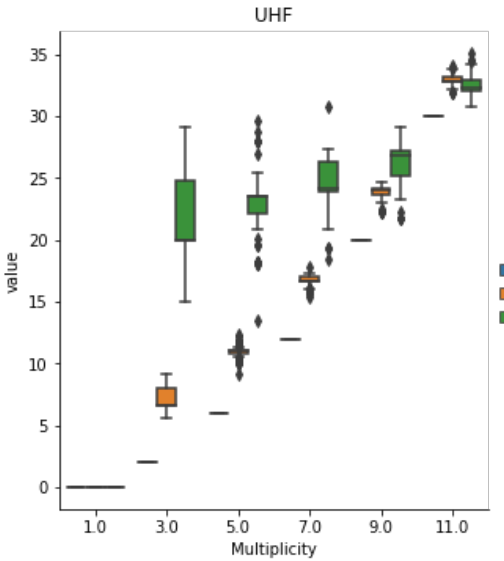
Exact Exchange in DFT

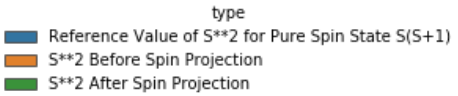
Jiri Hostas

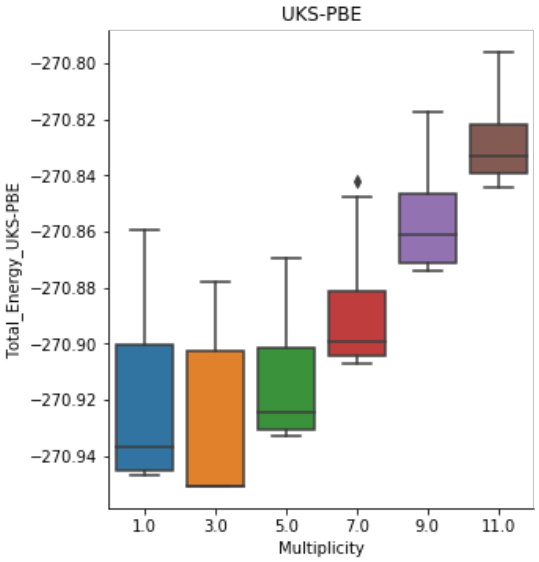
Spin contamination comparison

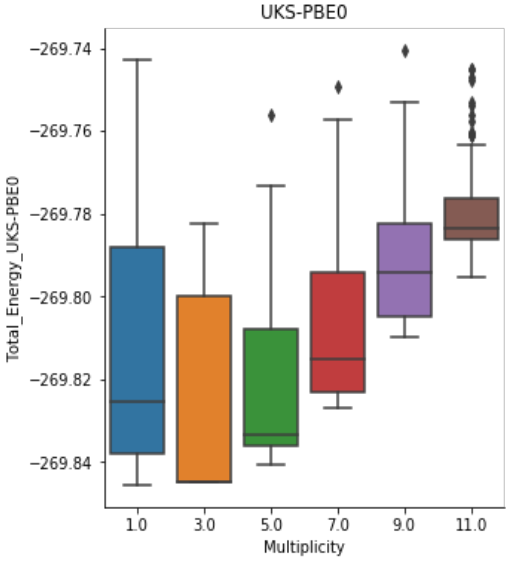


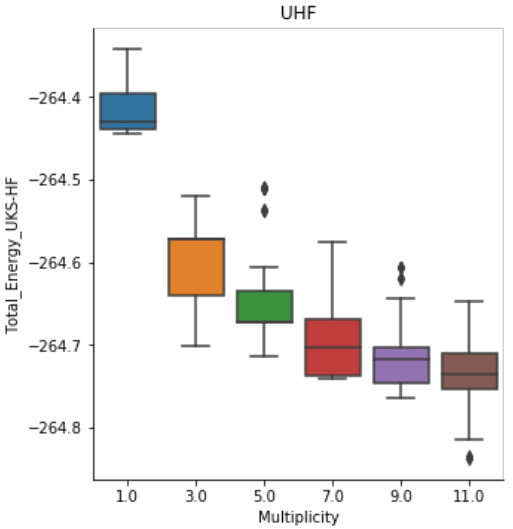


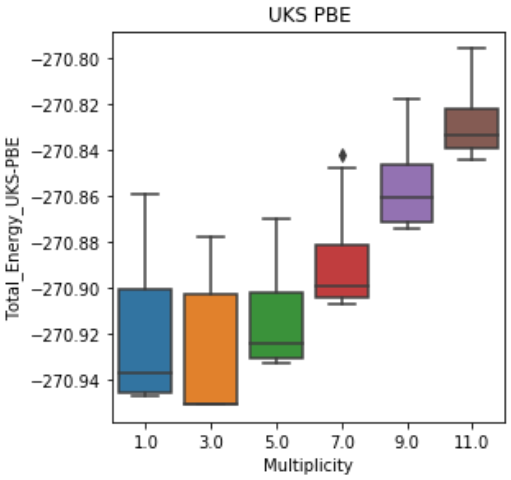


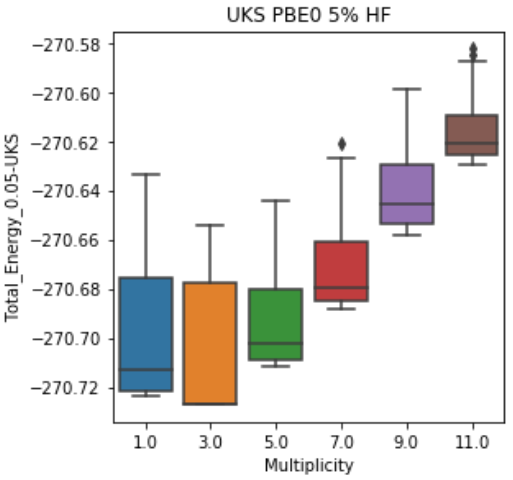


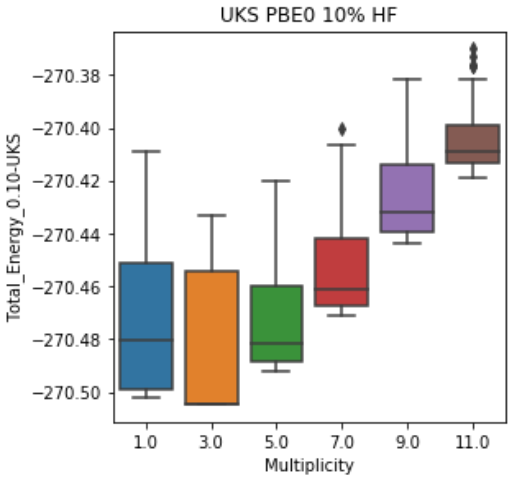


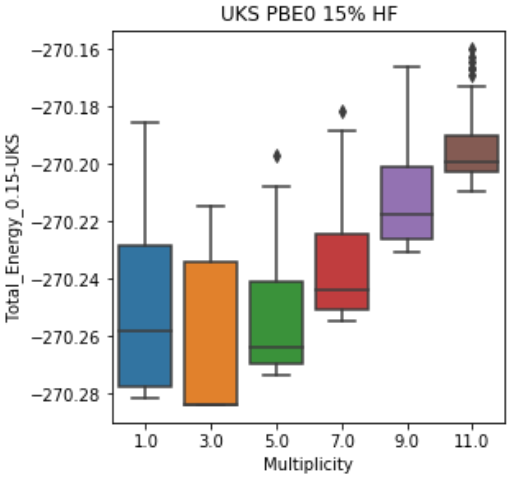





UKS PBE
Total_Energy_UKS-PBE
−270.80
−270.82
−270.84
−270.86
−270.88
−270.90
−270.92
−270.94
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity


UKS PBE0 5% HF
Total_Energy_0.05-UKS
−270.58
−270.60
−270.62
−270.64
−270.66
−270.68
−270.70
−270.72
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity


UKS PBE0 10% HF
Total_Energy_0.10-UKS
−270.38
−270.40
−270.42
−270.44
−270.46
−270.48
−270.50
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity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Total_Energy_0.15-UKS
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−270.20
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−270.26
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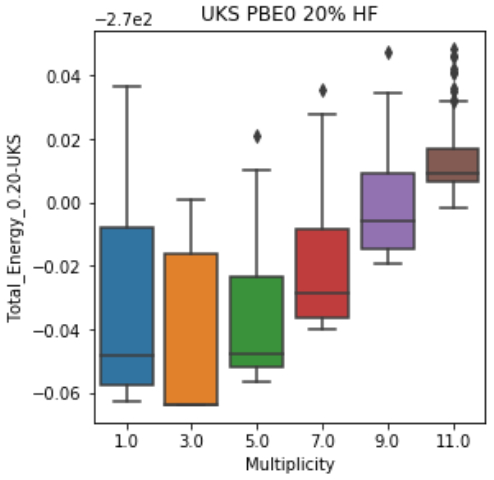
9.0
11.0
Multiplicity


−2.7e2
UKS PBE0 20% HF
Total_Energy_0.20-UKS
0.04
0.02
0.00
−0.02
−0.04
−0.06
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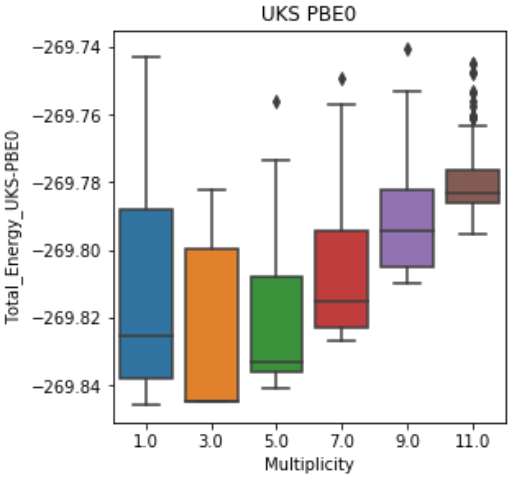
5.0
7.0
9.0
11.0
Multiplicity


UKS PBE0
Total_Energy_UKS-PBE0
−269.74
−269.76
−269.78
−269.80
−269.82
−269.84
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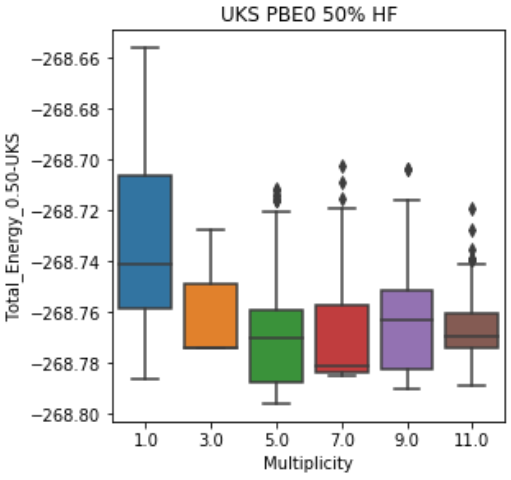
3.0
5.0
7.0
9.0
11.0
Multiplicity


UKS PBE0 50% HF
Total_Energy_0.50-UKS
−268.66
−268.68
−268.70
−268.72
−268.74
−268.76
−268.78
−268.80
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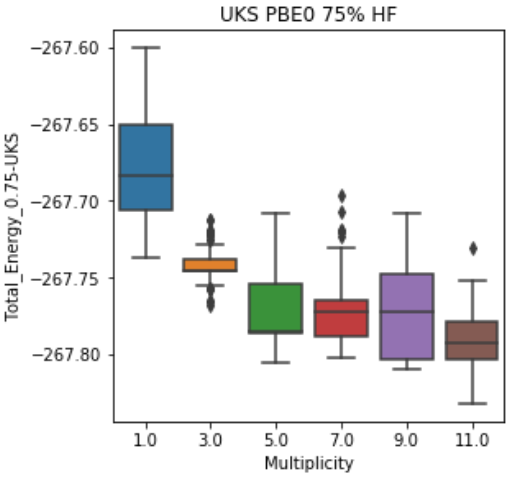
7.0
9.0
11.0
Multiplicity


UKS PBE0 75% HF
Total_Energy_0.75-UKS
−267.60
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−267.75
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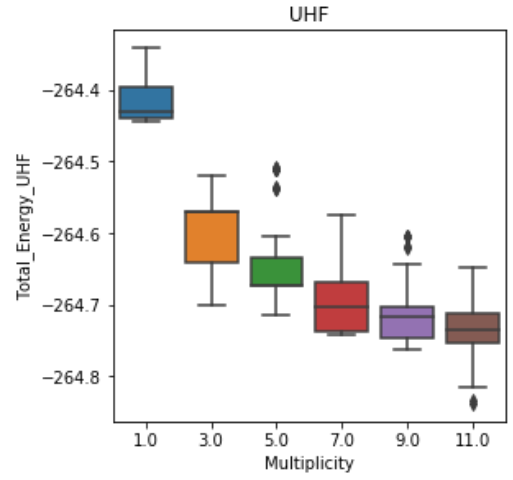
11.0
Multiplicity


UHF
Total_Energy_UHF
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−264.5
−264.6
−264.7
−264.8
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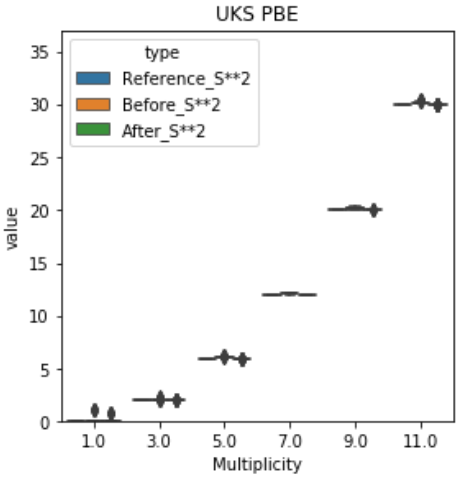
5.0
7.0
9.0
11.0
Multiplicity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After_S**2
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Multiplicity
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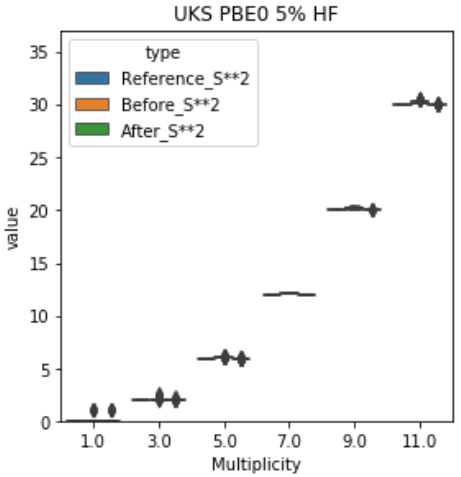
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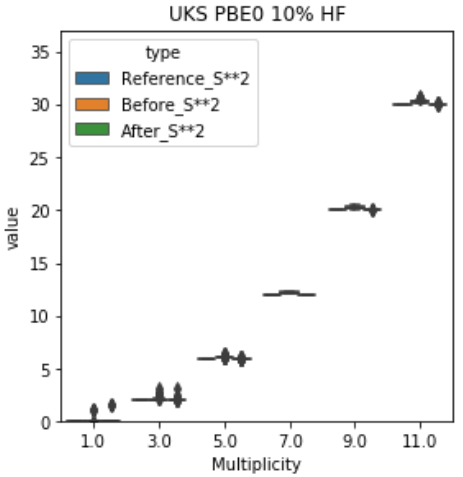
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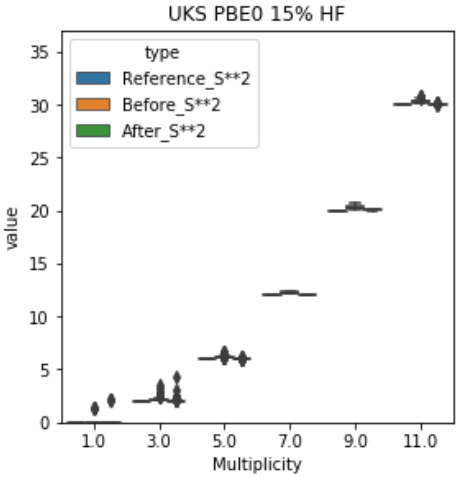
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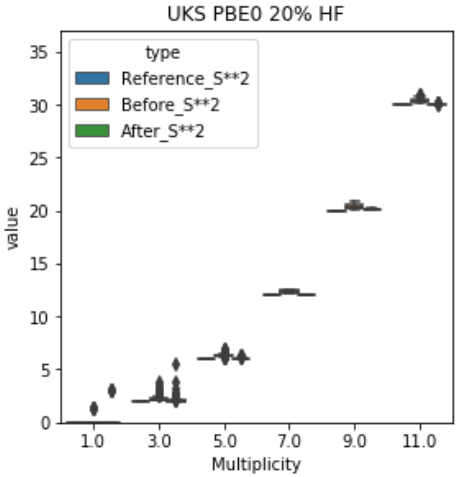
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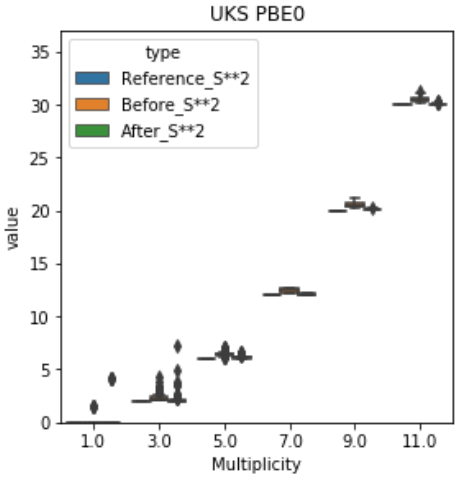
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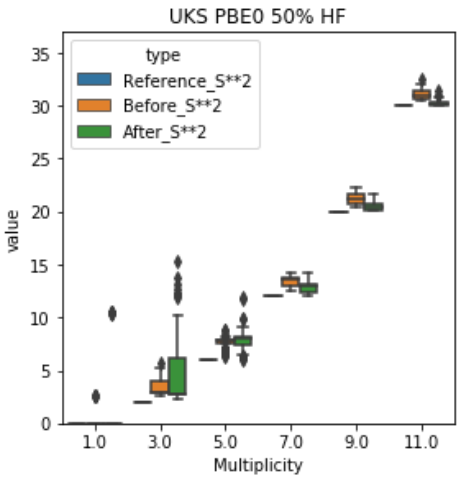
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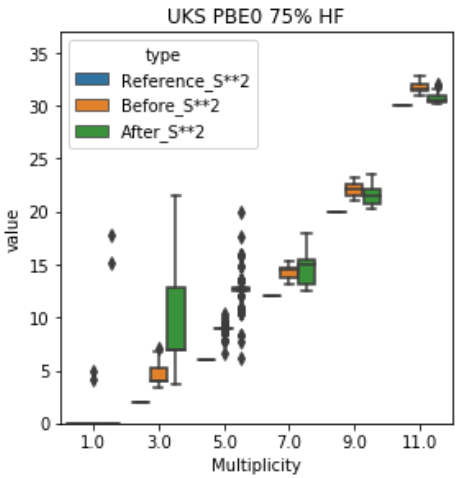
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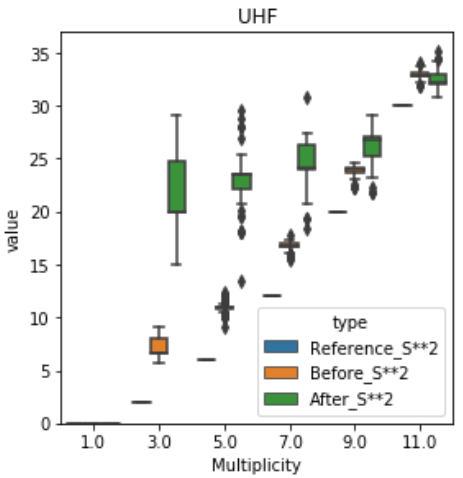
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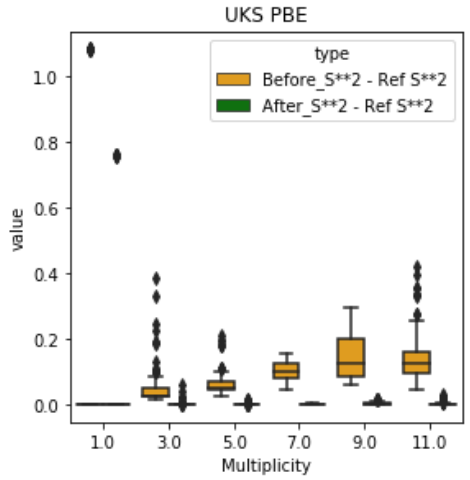
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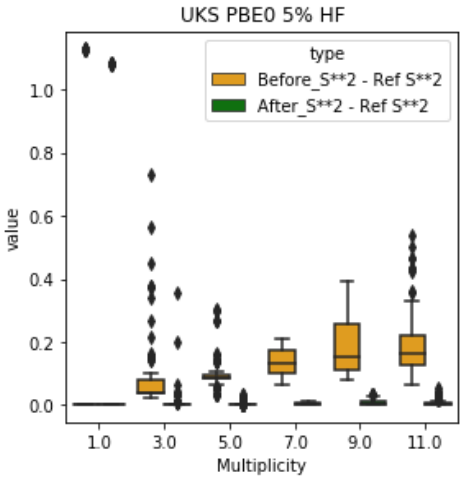
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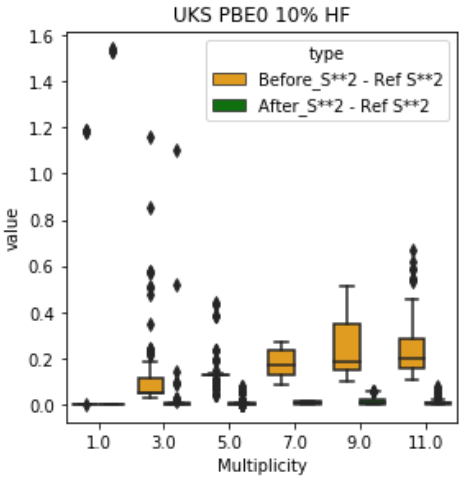
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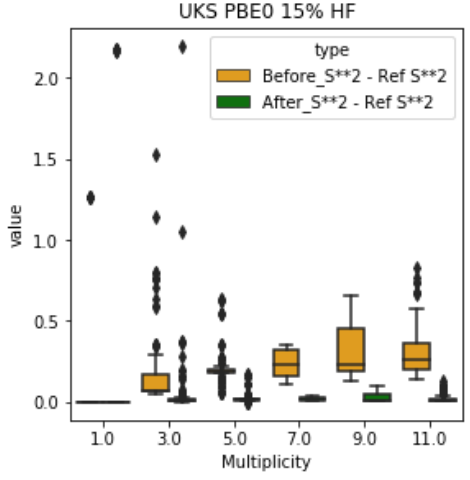
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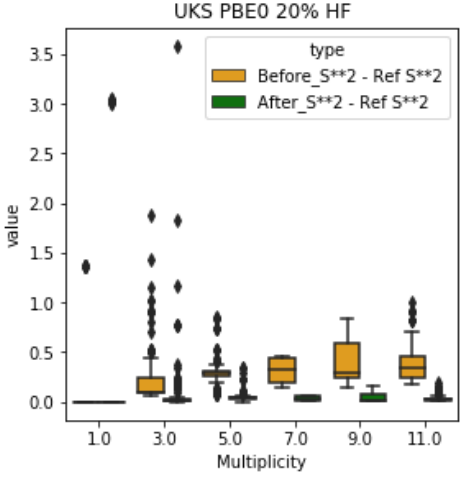
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After_S**2 - Ref S**2
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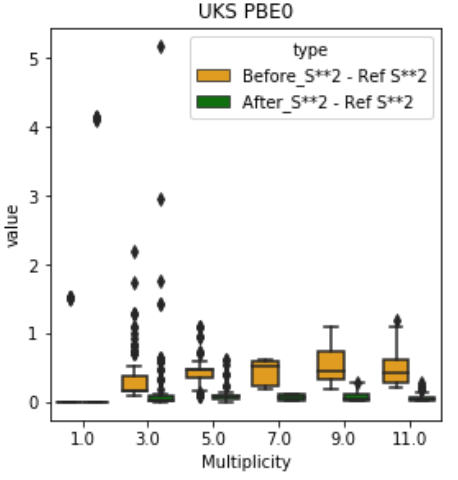
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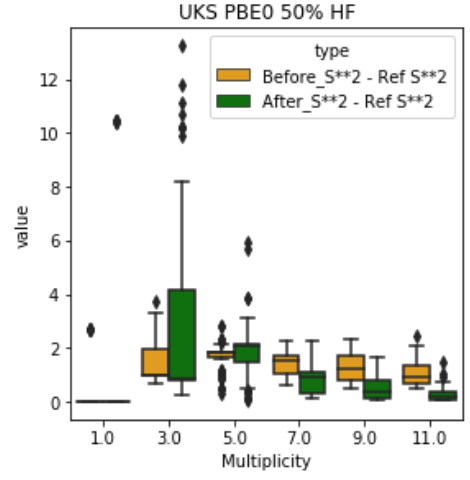
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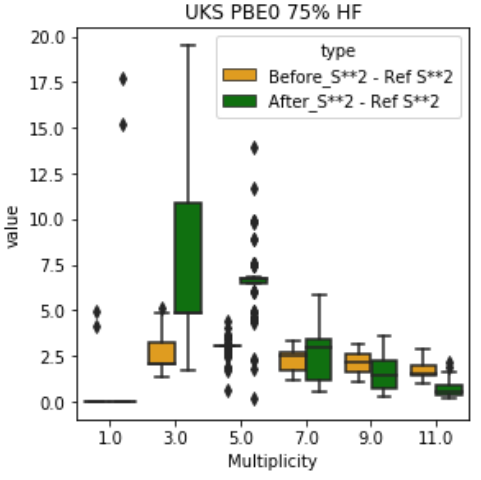
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After_S**2 - Ref S**2
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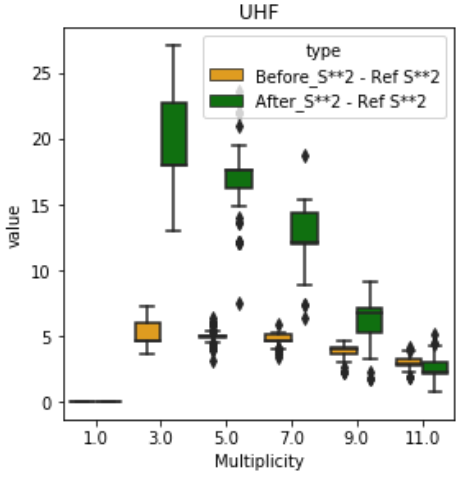
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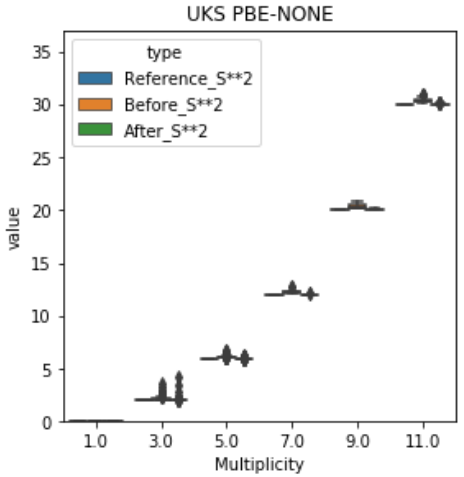
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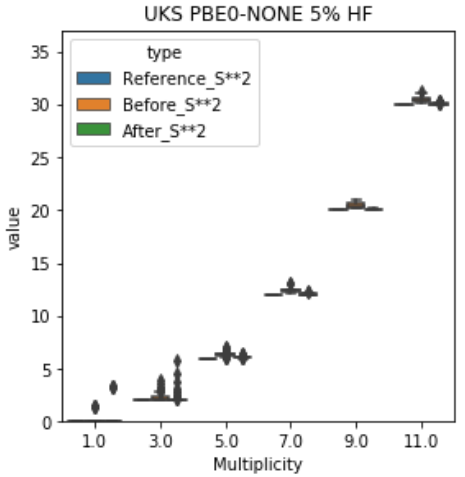
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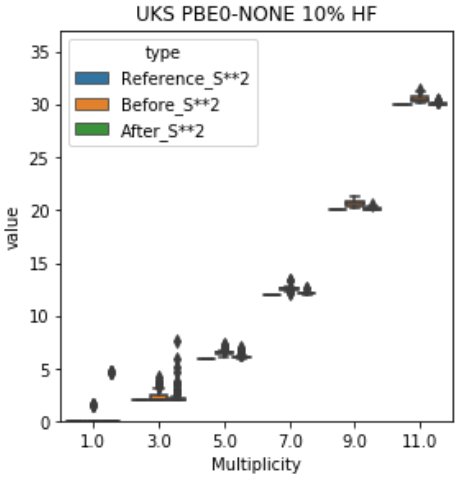
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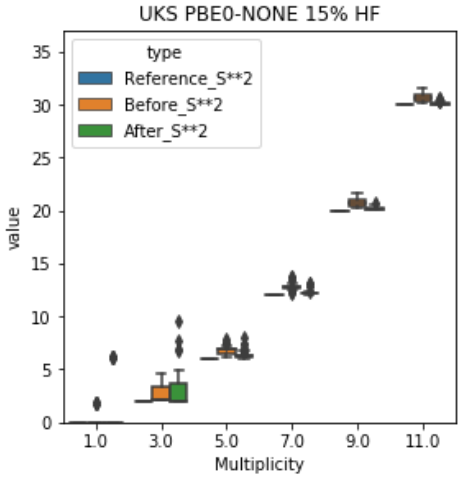
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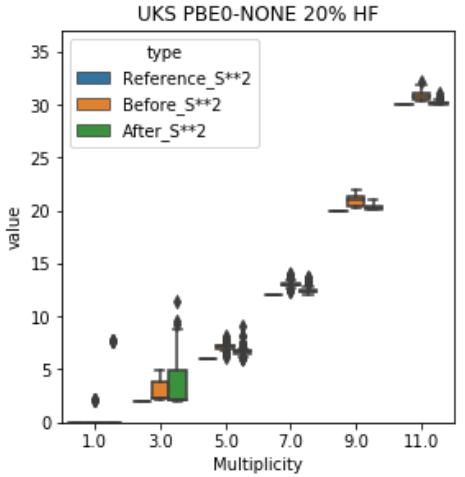
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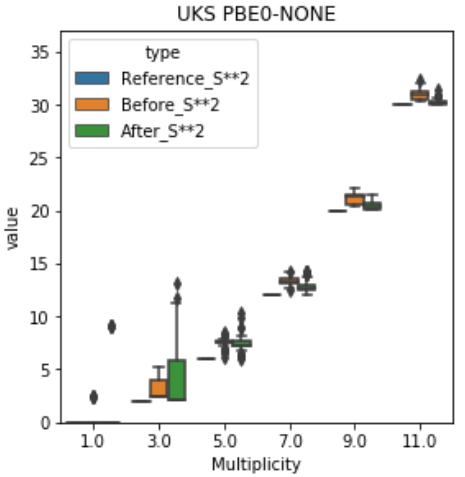
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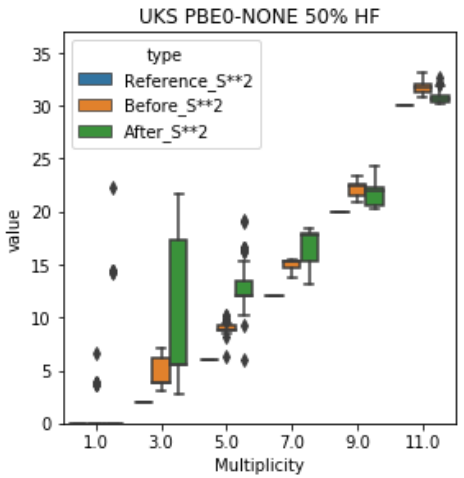
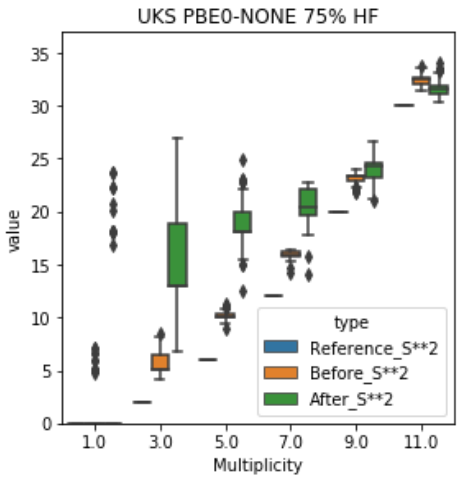
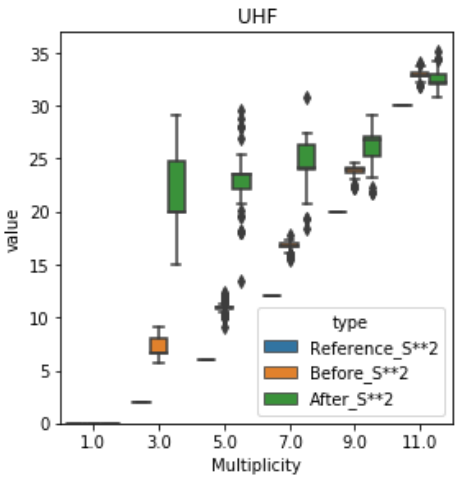
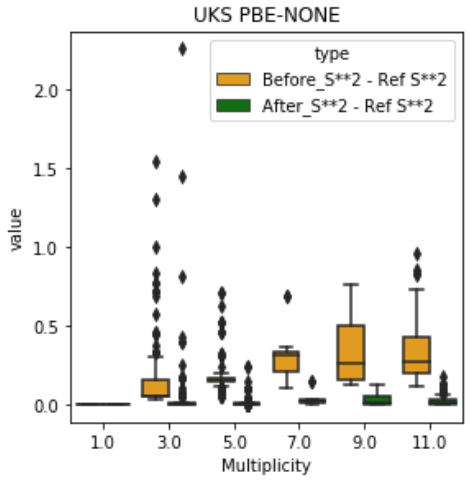
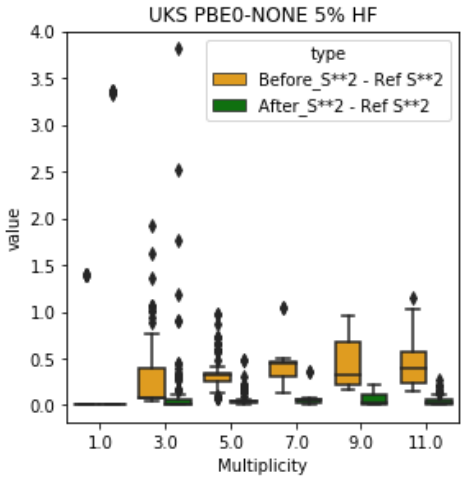
After_S**2
value
Multiplicity
1.0
3.0
5.0
7.0
9.0
11.0

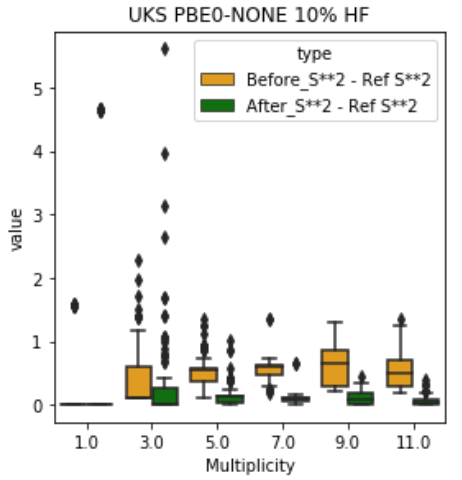

UKS PBE0-NONE 50% HF
type
Reference_S**2
Before_S**2
After_S**2
value
Multiplicity
1.0
3.0
5.0
7.0
9.0
11.0

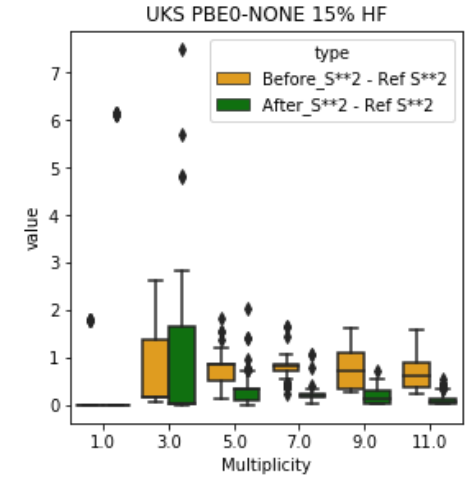

UKS PBE0-NONE 75% HF
type
Reference_S**2
Before_S**2
After_S**2
value
Multiplicity
1.0
3.0
5.0
7.0
9.0
11.0

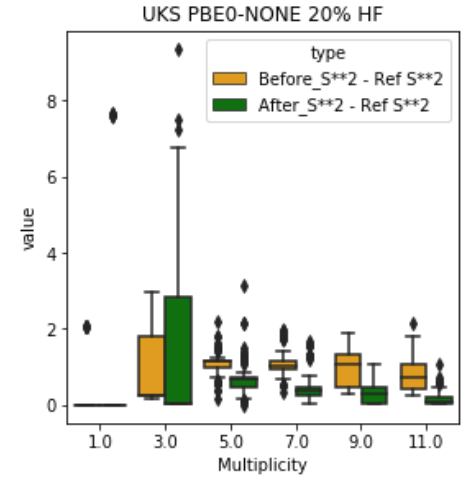

UHF
type
Reference_S**2
Before_S**2
After_S**2
value
Multiplicity
1.0
3.0
5.0
7.0
9.0
11.0

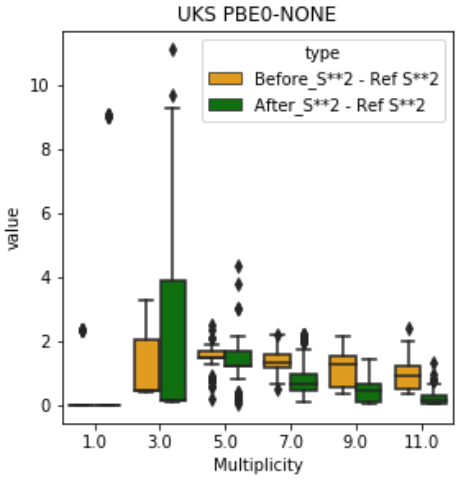

UKS PBE-NONE
type
Before_S**2 - Ref S**2
After_S**2 - Ref S**2
value
Multiplicity
1.0
3.0
5.0
7.0
9.0
11.0

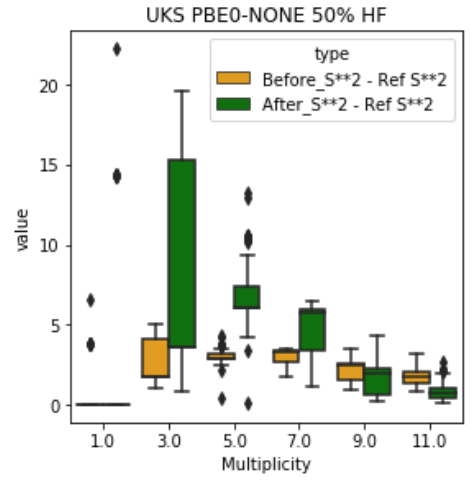

UKS PBE0-NONE 5% HF
type
Before_S**2 - Ref S**2
After_S**2 - Ref S**2
value
Multiplicity
1.0
3.0
5.0
7.0
9.0
11.0

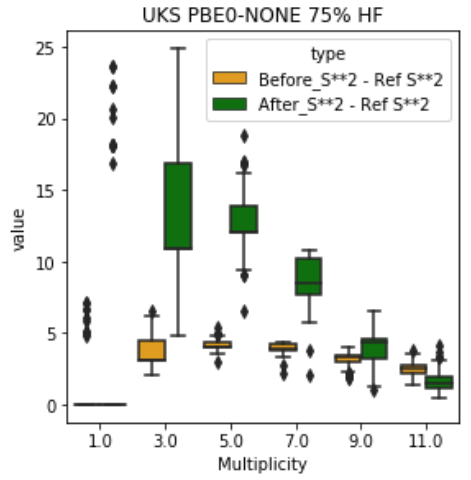

UKS PBE0-NONE 10% HF
type
Before_S**2 - Ref S**2
After_S**2 - Ref S**2
value
Multiplicity
1.0
3.0
5.0
7.0
9.0
11.0

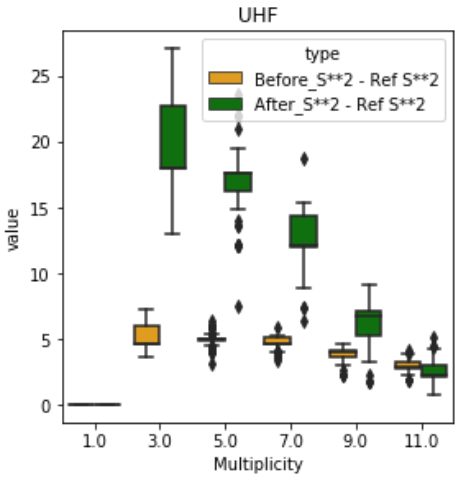

UKS PBE0-NONE 15% HF
type
Before_S**2 - Ref S**2
After_S**2 - Ref S**2
value
Multiplicity
1.0
3.0
5.0
7.0
9.0
11.0

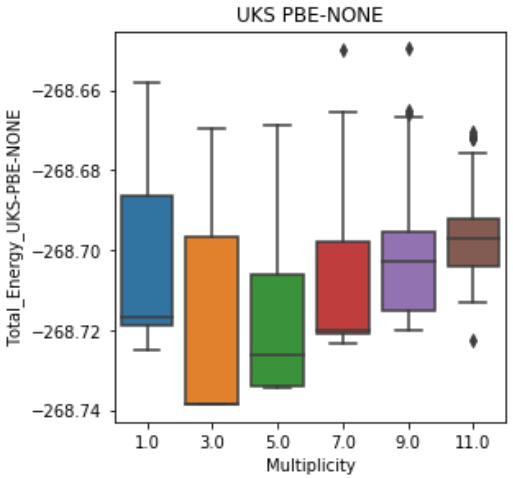

UKS PBE0-NONE 20% HF
type
Before_S**2 - Ref S**2
After_S**2 - Ref S**2
value
Multiplicity
1.0
3.0
5.0
7.0
9.0
11.0

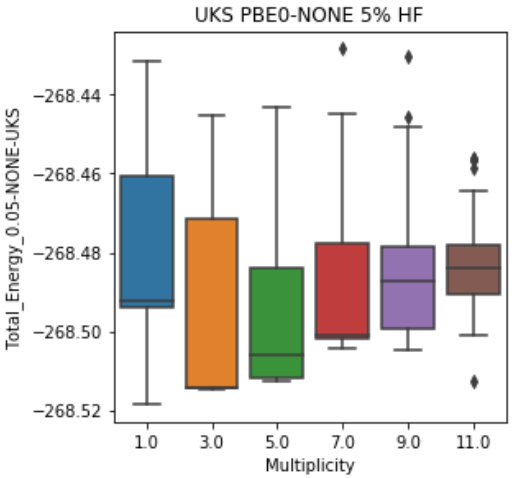

UKS PBE0-NONE
type
Before_S**2 - Ref S**2
After_S**2 - Ref S**2
value
Multiplicity
1.0
3.0
5.0
7.0
9.0
11.0

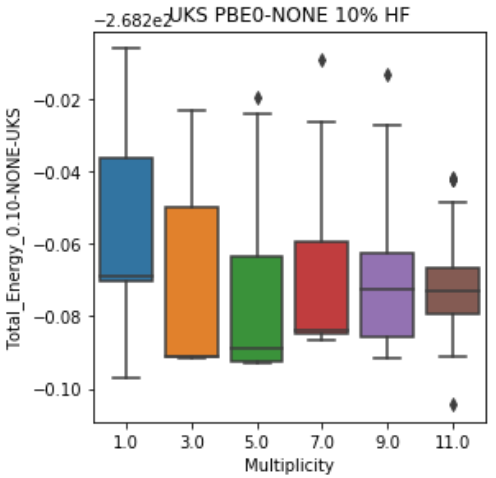

UKS PBE0-NONE 50% HF
type
Before_S**2 - Ref S**2
After_S**2 - Ref S**2
value
Multiplicity
1.0
3.0
5.0
7.0
9.0
11.0

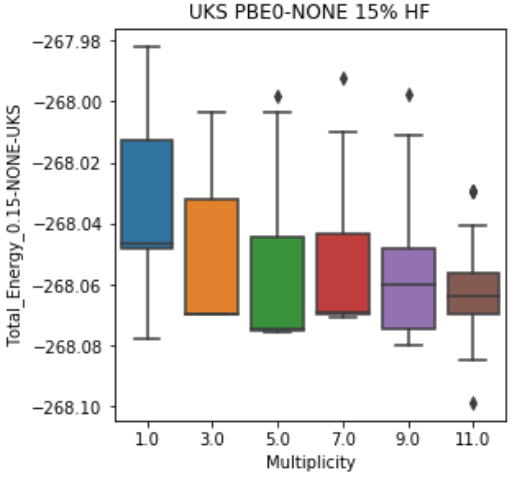

UKS PBE0-NONE 75% HF
type
Before_S**2 - Ref S**2
After_S**2 - Ref S**2
value
Multiplicity
1.0
3.0
5.0
7.0
9.0
11.0

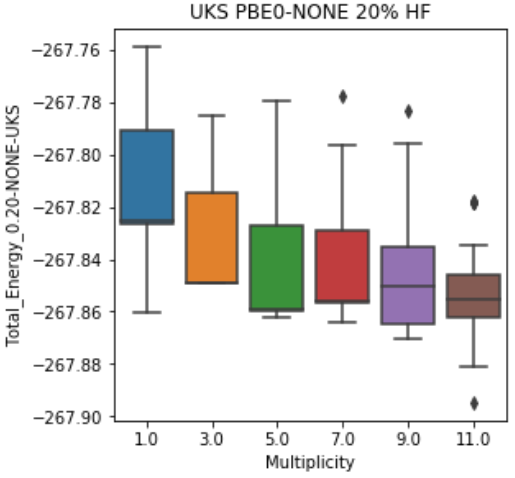

UHF
type
Before_S**2 - Ref S**2
After_S**2 - Ref S**2
value
Multiplicity
1.0
3.0
5.0
7.0
9.0
11.0

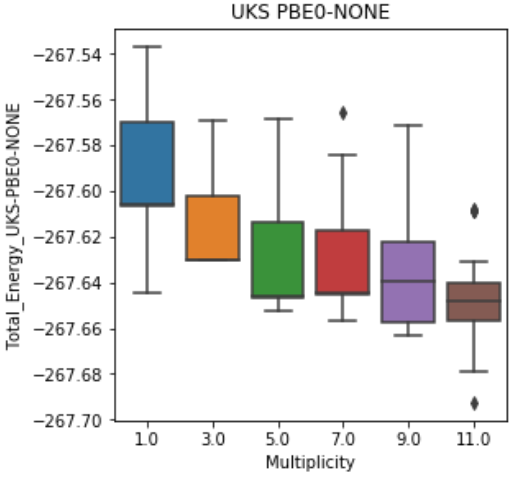

UKS PBE-NONE
Total_Energy_UKS-PBE-NONE
−268.66
−268.68
−268.70
−268.72
−268.74
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

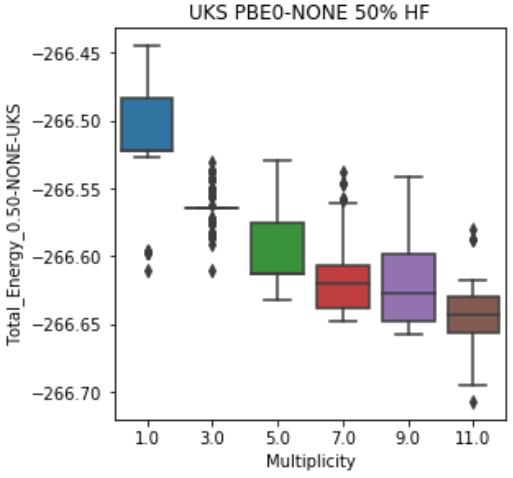

UKS PBE0-NONE 5% HF
Total_Energy_0.05-NONE-UKS
−268.44
−268.46
−268.48
−268.50
−268.52
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

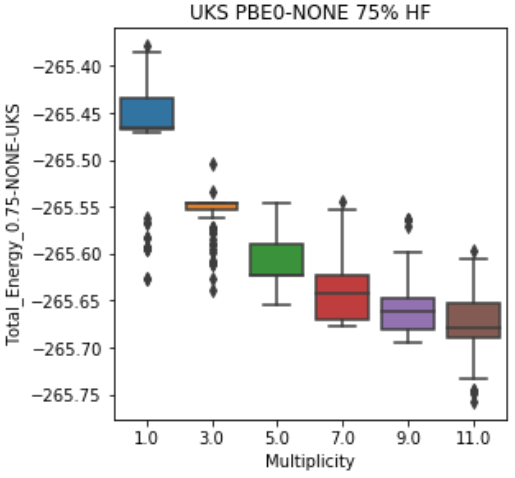

−2.682e2
UKS PBE0-NONE 10% HF
Total_Energy_0.10-NONE-UKS
−0.02
−0.04
−0.06
−0.08
−0.10
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

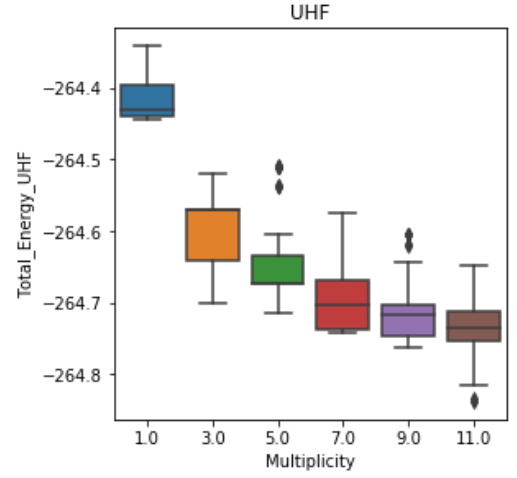

UKS PBE0-NONE 15% HF
Total_Energy_0.15-NONE-UKS
−267.98
−268.00
−268.02
−268.04
−268.06
−268.08
−268.10
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity


UKS PBE0-NONE 20% HF
Total_Energy_0.20-NONE-UKS
−267.76
−267.78
−267.80
−267.82
−267.84
−267.86
−267.88
−267.90
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

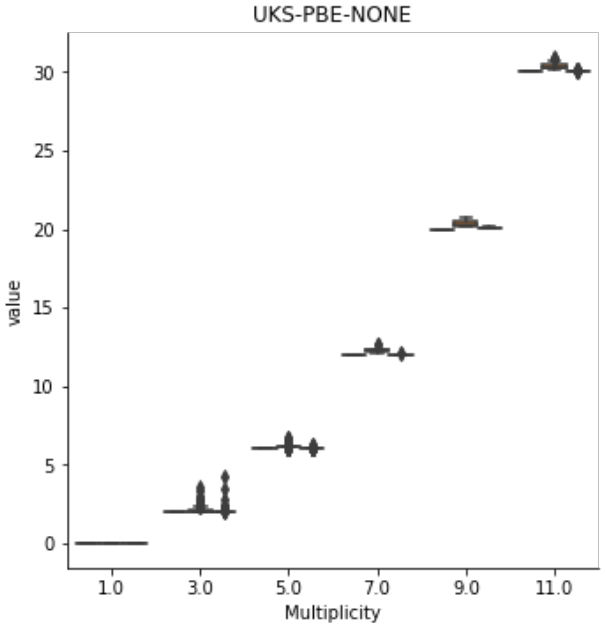

UKS PBE0-NONE
Total_Energy_UKS-PBE0-NONE
−267.54
−267.56
−267.58
−267.60
−267.62
−267.64
−267.66
−267.68
−267.70
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

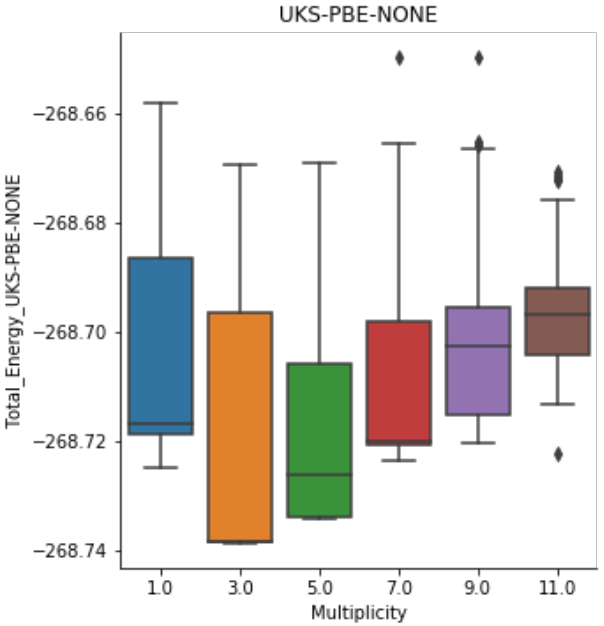

UKS PBE0-NONE 50% HF
Total_Energy_0.50-NONE-UKS
−266.45
−266.50
−266.55
−266.60
−266.65
−266.70
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

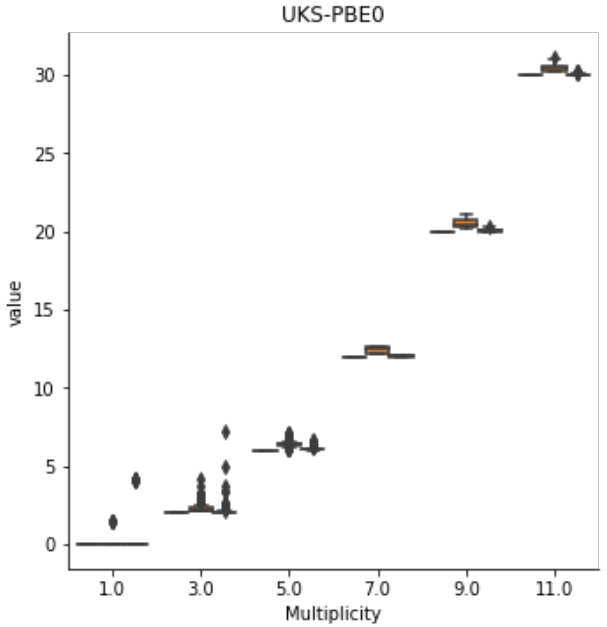

UKS PBE0-NONE 75% HF
Total_Energy_0.75-NONE-UKS
−265.40
−265.45
−265.50
−265.55
−265.60
−265.65
−265.70
−265.75
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

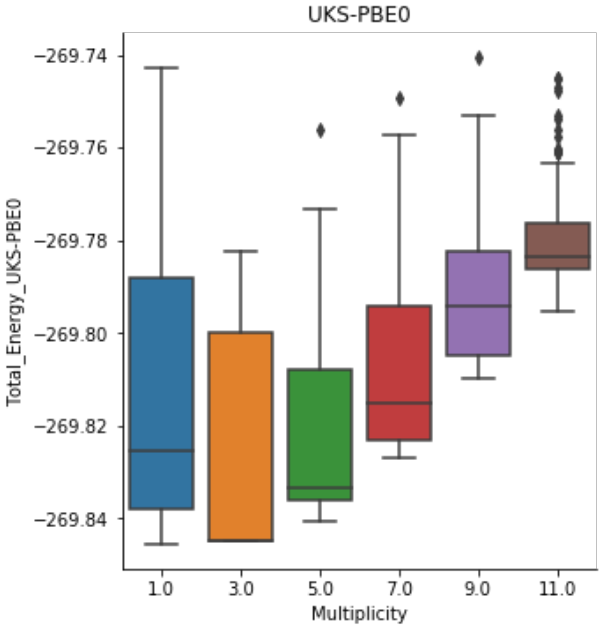

UHF
Total_Energy_UHF
−264.4
−264.5
−264.6
−264.7
−264.8
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

Is PBE-NONE similar to PBE0 ?

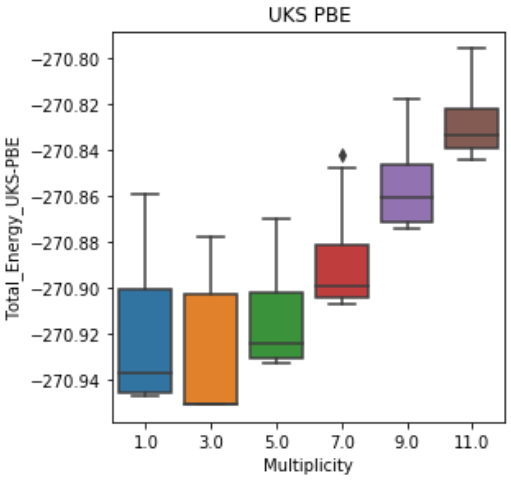


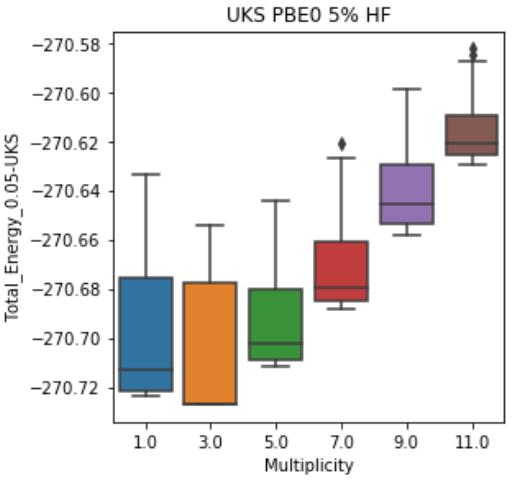


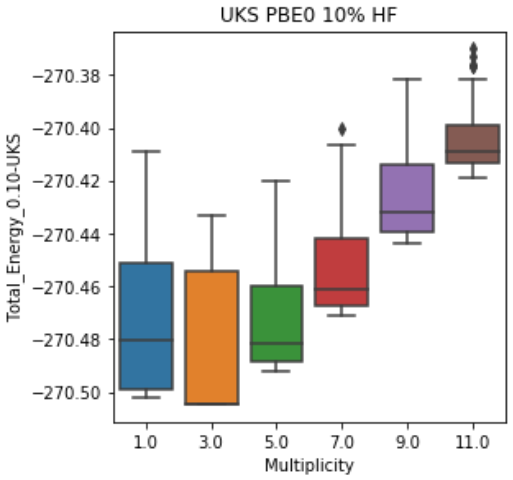


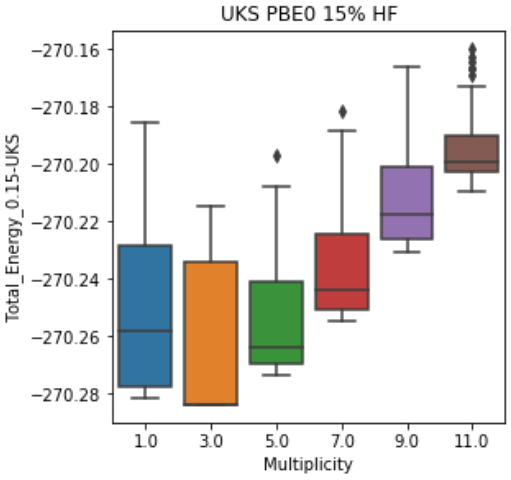


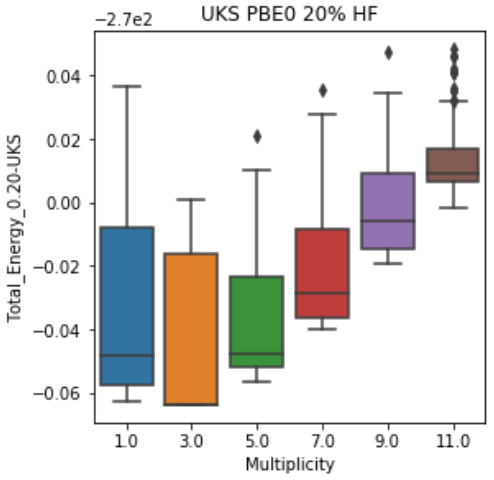
ROKS

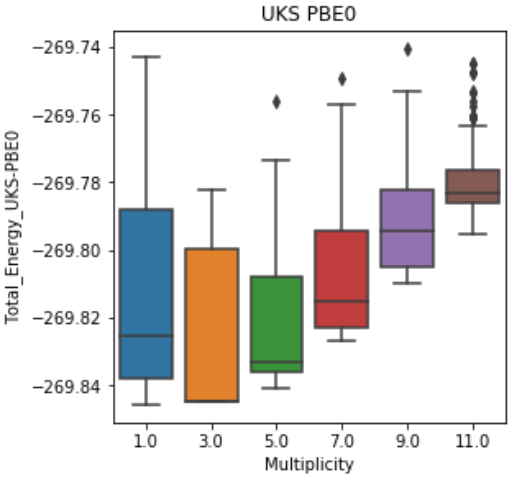

UKS PBE
Total_Energy_UKS-PBE
−270.80
−270.82
−270.84
−270.86
−270.88
−270.90
−270.92
−270.94
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

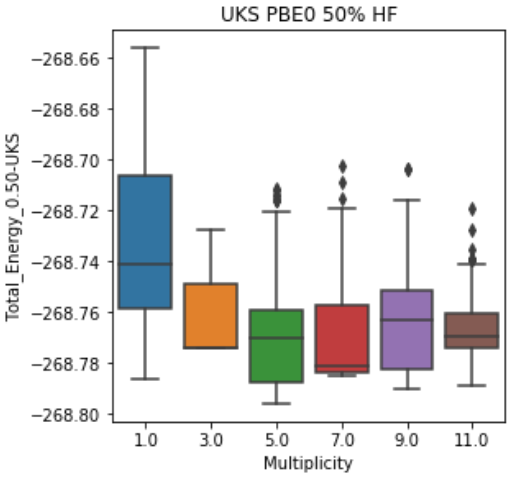

UKS PBE0 5% HF
Total_Energy_0.05-UKS
−270.58
−270.60
−270.62
−270.64
−270.66
−270.68
−270.70
−270.72
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

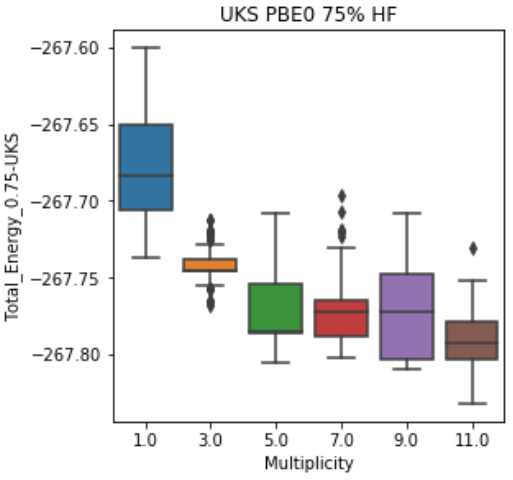

UKS PBE0 10% HF
Total_Energy_0.10-UKS
−270.38
−270.40
−270.42
−270.44
−270.46
−270.48
−270.50
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

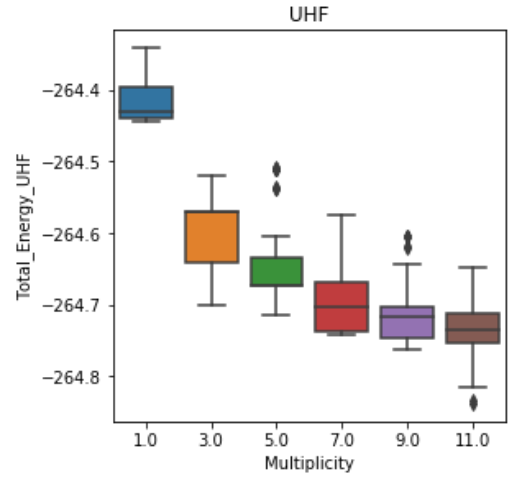

UKS PBE0 15% HF
Total_Energy_0.15-UKS
−270.16
−270.18
−270.20
−270.22
−270.24
−270.26
−270.28
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

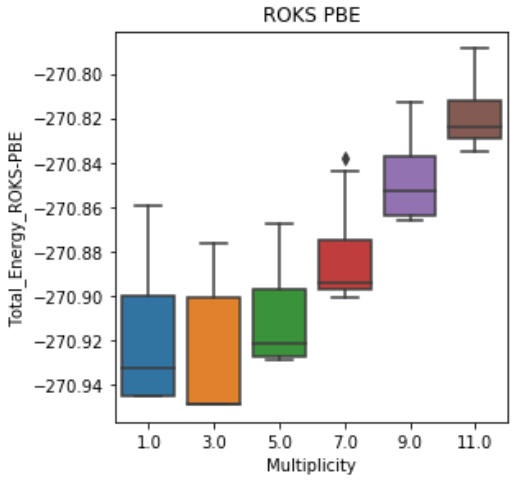

−2.7e2
UKS PBE0 20% HF
Total_Energy_0.20-UKS
0.04
0.02
0.00
−0.02
−0.04
−0.06
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

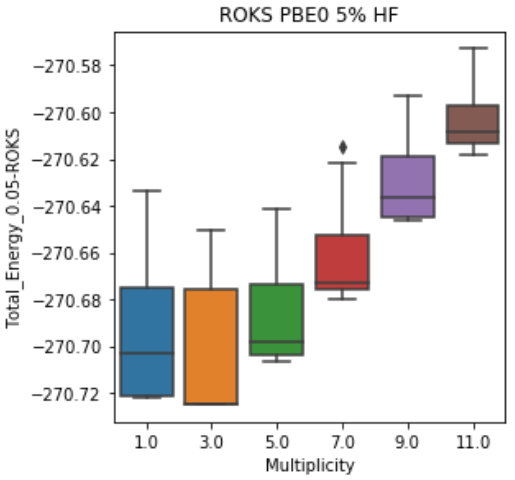

UKS PBE0
Total_Energy_UKS-PBE0
−269.74
−269.76
−269.78
−269.80
−269.82
−269.84
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

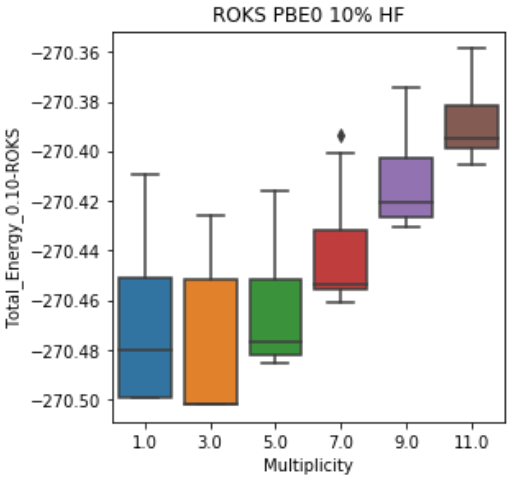

UKS PBE0 50% HF
Total_Energy_0.50-UKS
−268.66
−268.68
−268.70
−268.72
−268.74
−268.76
−268.78
−268.80
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

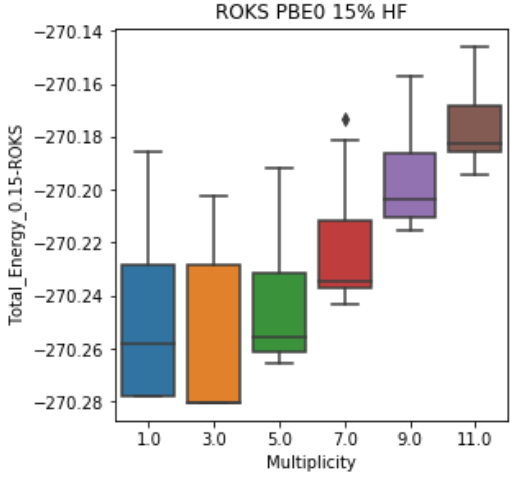

UKS PBE0 75% HF
Total_Energy_0.75-UKS
−267.60
−267.65
−267.70
−267.75
−267.80
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

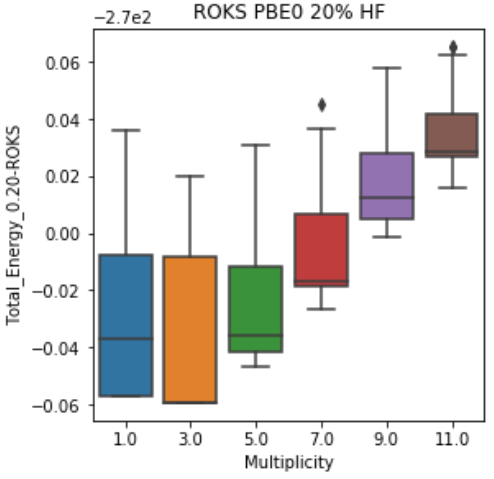

UHF
Total_Energy_UHF
−264.4
−264.5
−264.6
−264.7
−264.8
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

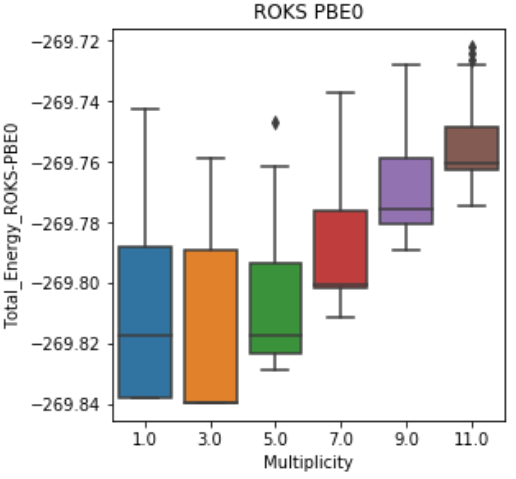

ROKS PBE
Total_Energy_ROKS-PBE
−270.80
−270.82
−270.84
−270.86
−270.88
−270.90
−270.92
−270.94
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

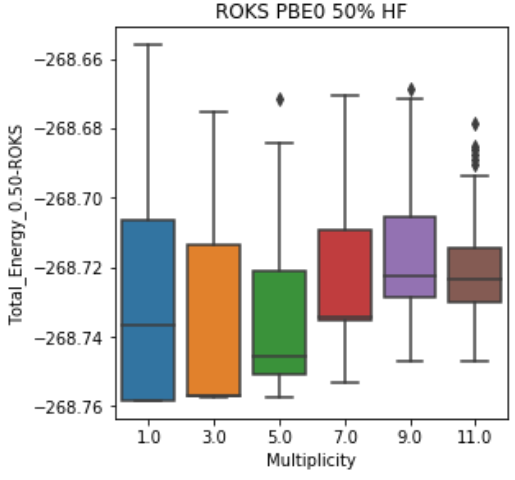

ROKS PBE0 5% HF
Total_Energy_0.05-ROKS
−270.58
−270.60
−270.62
−270.64
−270.66
−270.68
−270.70
−270.72
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

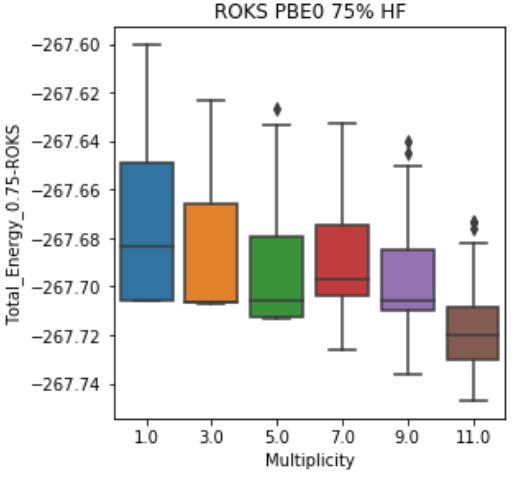

ROKS PBE0 10% HF
Total_Energy_0.10-ROKS
−270.36
−270.38
−270.40
−270.42
−270.44
−270.46
−270.48
−270.50
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

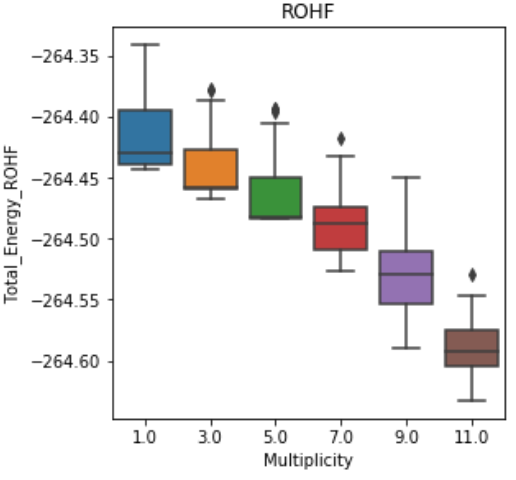

ROKS PBE0 15% HF
Total_Energy_0.15-ROKS
−270.14
−270.16
−270.18
−270.20
−270.22
−270.24
−270.26
−270.28
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity

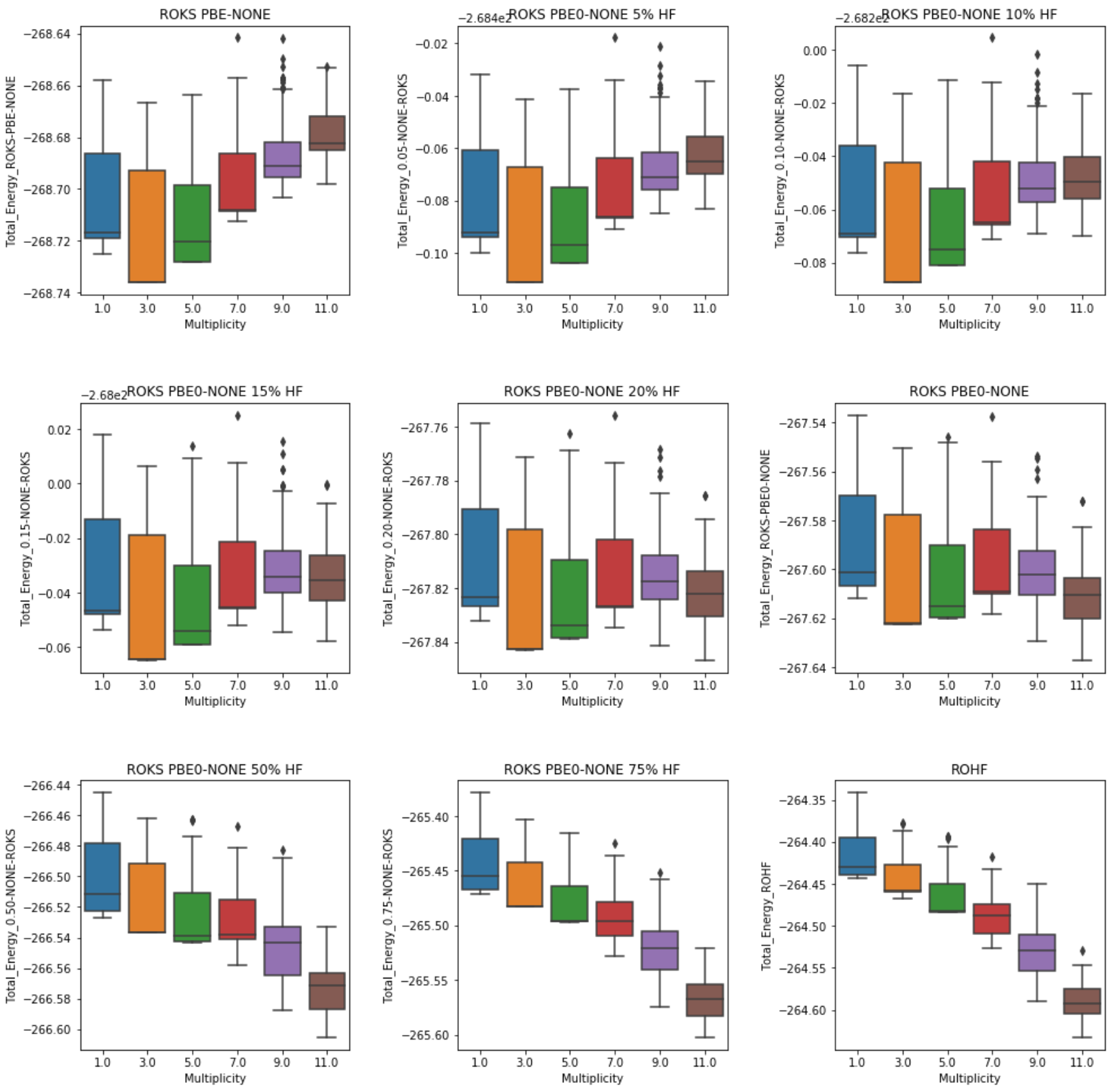

−2.7e2
ROKS PBE0 20% HF
Total_Energy_0.20-ROKS
0.06
0.04
0.02
0.00
−0.02
−0.04
−0.06
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity


ROKS PBE0
Total_Energy_ROKS-PBE0
−269.72
−269.74
−269.76
−269.78
−269.80
−269.82
−269.84
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity


ROKS PBE0 50% HF
Total_Energy_0.50-ROKS
−268.66
−268.68
−268.70
−268.72
−268.74
−268.76
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity


ROKS PBE0 75% HF
Total_Energy_0.75-ROKS
−267.60
−267.62
−267.64
−267.66
−267.68
−267.70
−267.72
−267.74
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity


ROHF
Total_Energy_ROHF
−264.35
−264.40
−264.45
−264.50
−264.55
−264.60
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity


ROKS PBE-NONE
Total_Energy_ROKS-PBE-NONE
−268.64
−268.66
−268.68
−268.70
−268.72
−268.74
1.0
3.0
5.0
7.0
9.0
11.0
Multiplicity
−2.684e2
ROKS PBE0-NONE 5% HF
Total_Energy_0.05-NONE-ROKS
−0.02
−0.04
−0.06
−0.08
−0.10
Multiplicity
−2.682e2
ROKS PBE0-NONE 10% HF
Total_Energy_0.10-NONE-ROKS
0.00
−0.02
−0.04
−0.06
−0.08
Multiplicity
−2.68e2
ROKS PBE0-NONE 15% HF
Total_Energy_0.15-NONE-ROKS
0.02
0.00
−0.02
−0.04
−0.06
Multiplicity
ROKS PBE0-NONE 20% HF
Total_Energy_0.20-NONE-ROKS
−267.76
−267.78
−267.80
−267.82
−267.84
Multiplicity
ROKS PBE0-NONE
Total_Energy_ROKS-PBE0-NONE
−267.54
−267.56
−267.58
−267.60
−267.62
−267.64
Multiplicity
ROKS PBE0-NONE 50% HF
Total_Energy_0.50-NONE-ROKS
−266.44
−266.46
−266.48
−266.50
−266.52
−266.54
−266.56
−266.58
−266.60
Multiplicity
ROKS PBE0-NONE 75% HF
Total_Energy_0.75-NONE-ROKS
−265.40
−265.45
−265.50
−265.55
−265.60
Multiplicity
ROHF
Total_Energy_ROHF
−264.35
−264.40
−264.45
−264.50
−264.55
−264.60
Multiplicity