nline average vres iteration 240 Iteration for first e-10

Iterations 236-240

4 1.25e-11 +-.236e-11 1.060e-11 42

5 1.30e-11 +-.2652e-11 1.162 e-11 42

6 1.29e-11+-.611e-11 1.494e-11 79

7 1.15 e-11 +-.0896e-11 1.19 e-11 40

8 1.23e-11+-.327e-11 1.187e-11 37

9 1.23e-11 +-.284e-11 1.266 e-11 42

10 1.19e-11+- .180e-11 9.965 e-12 42

Diemix average vres iteration 240 Iteration for first e-10

0.2 9.29 e-12+-3.59e-12 7.278 e-12 96

0.4 6.738 e-12+-3.54e-12 1.249 e-11 54

0.6 5.55e-12+-2.52e-12 1.098 e-11 43

0.8 7.446 e-12+-2.91e-12 6.559 e-12 27

1,0 . 7.092 e-12+-3.47e-12 6.484 e-12 30

diemac average vres iteration 240 Iteration for first e-10

diemac+5 1.28 e-11 +-.527e-11 8.415 e-12 85

diemac+6 1.72e-11+-.444e-11 1.572 e-11 81

diemac+7 1.72e-11 +-.444e-11 1.572 e-11 81

diemac+8 1.72e-11 +-.444e-11 1.572 e-11 81

diemac+9 1.72e-11+-.444e-11 1.572 e-11 81

Diemac4dielng0.2 average vres iteration 240 Iteration for first e-10

Iterations 236-240

Diemac 4 dielng .2 1.33 e-11+-.377e-11 1.555 e-11 47

iprcel average vres iteration 240 Iteration for first e-10

Iterations 236-240

1. 4.14e+2 3.942e+2

25 1.09e-11 1.016e-11 83

35 1.57e-11 1.923e-11 74

41 1.64.67e-11 9.390e-12 42

45 1.78e-11 2.200e-11 47

55 3.88e-11 4.704e-11 57

65 5.47e+3 5.466e+3

145 1.62e-11 1.609e-11 46

dielng average vres iteration 240 Iteration for first e-10

Iterations 236-240

.2 1.41e-11 1.459e-11 68

.4 3.01e-11 2.570e-11 49

.6 1.79e-11.309e-11 2.200e-11 47

.8 1.79e-11.309e-11 2.200e-11 47

1.0 1.79e-11.309e-11 2.200e-11 47





The work function for the different values of tolvrs is.

WF = = 0.2098429 Ha = 5.710116 eV tolvrs = 1d-4

= 0.20984208 Ha = 5.710094 eV tolvrs = 1d-5

= 0.20984228 Ha = 5.710099 eV tolvrs = 1d-6

= 0.209842067 Ha = 5.7100932 eV tolvrs = 1d-7

= 0.209842067 Ha = 5.710093 eV tolvrs = 1d-8

= 0.2098442 Ha = 5.71015 eV tolvrs = 1e-9

= 0.2098586 Ha = 5.7105431 eV tolvrs = 1e-10

= 0.20984409 Ha = 5.710148 eV tolvrs = 1e-11

= 0.20984211 Ha = 5.710094 eV tolvrs = 1e-12

= 0.209846326 Ha = 5.710209 eV tolvrs = 1e-13

Subtracting the largest value of the WF at tolvrs = 1d-10 (5.7105431 eV) from the others we get

Difference in WF = -4.271d-4 tolvrs = 1d-4

-4.491d-4 tolvrs = 1d-5

-4.441d-4 tolvrs = 1d-6

-4.449d-4 tolvrs = 1d-7

-4.501d-4 tolvrs = 1e-8

-3.931d-4 tolvrs = 1d-9

0.000 tolvrs = 1e-10

-3.951d-4 tolvrs = 1d-11

-4.491d-4 tolvrs = 1d-12

-3.341d-4 tolvrs = 1d-13

WFavg = 4.207d-4±0.396d-4 eV => ±6.95d-4 % error (.396d-4/5.711S)\*100

Plotting the differences of the work function vs. tolvrs on a linear-log plot we have

