[Electronic supporting information]

**Influence of water contamination on the sputtering of silicon with low energy argon ions investigated by Molecular Dynamics simulations.**

Grégoire R.N. Defoort-Levkov\*1,2, Alan Bahm 3, Patrick Philipp \*1

1 – Advanced Instrumentation for Nano-Analytics (AINA), Materials Research and Technology Department (MRT), Luxembourg Institute of Science and Technology (LIST), 4422 Belvaux, Luxembourg.

2 – University of Luxembourg, 4365 Esch-sur-Alzette, Luxembourg.

3 – Thermo Fisher Scientific, Hillsboro, OR, 97124, USA

Email: Patrick Philipp – Patrick.philipp@list.lu

\* Corresponding author

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**ReaxFF Potential**

**Table 1.** Force field parameters, from “Oxidation of Silicon Carbide by O2 and H2O: A ReaxFF Reactive Molecular Dynamics Study, Part I” by David A. Newsome. et. al. - *J. Phys. Chem. C* 2012, 116, 30, 16111–16121.

**Graph 1.** Ar – Si Potential, full potential



**Graph 2.** Ar – Si Potential, focused part of the potential

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**Graph 3.** Ar – O Potential, full potential.

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**Graph 4.** Ar – O Potential, focused part of the potential

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**Graph 5**. Ar – H Potential, full potential.

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**Graph 6**. Ar – H Potential, focused part of the potential

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**Graph 8**. Ar – Ar Potential, focused part of the potential

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**G(r) per slab and grouping details**

**Graph 9** Detailed g(r) for each slab for 100 ev, 0° and 500 bombardments

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**Graph 10** Detailed g(r) for each slab for 100 ev, 45° and 500 bombardments

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**Graph 11** Detailed g(r) for each slab for 100 ev, 75° and 500 bombardments

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**ReaxFF potential**   
**Table 1**. Details of the ReaxFF potential used in the simulations.

Reactive MD-force field: c/h/o/Si/C August 3  
39 ! Number of general parameters   
50.0000 !Overcoordination parameter   
9.5469 !Overcoordination parameter   
26.5405 !Valency angle conjugation parameter   
1.5105 !Triple bond stabilisation parameter   
6.6630 !Triple bond stabilisation parameter   
0.0000 !C2-correction   
1.0588 !Undercoordination parameter   
4.6000 !Triple bond stabilisation parameter   
12.1176 !Undercoordination parameter   
13.3056 !Undercoordination parameter   
-70.1292 !Triple bond stabilization energy   
0.0000 !Lower Taper-radius   
10.0000 !Upper Taper-radius   
2.8793 !Not used   
33.8667 !Valency undercoordination   
6.0891 !Valency angle/lone pair parameter   
1.0563 !Valency angle   
2.0384 !Valency angle parameter   
6.1431 !Not used   
6.9290 !Double bond/angle parameter   
0.3989 !Double bond/angle parameter: overcoord   
3.9954 !Double bond/angle parameter: overcoord   
-2.4837 !Not used   
5.7796 !Torsion/BO parameter   
10.0000 !Torsion overcoordination   
1.9487 !Torsion overcoordination   
-1.2327 !Conjugation 0 (not used)   
2.1645 !Conjugation   
1.5591 !vdWaals shielding   
0.1000 !Cutoff for bond order (\*100)   
2.1365 !Valency angle conjugation parameter   
0.6991 !Overcoordination parameter   
50.0000 !Overcoordination parameter   
1.8512 !Valency/lone pair parameter   
0.5000 !Not used   
20.0000 !Not used   
5.0000 !Molecular energy (not used)   
0.0000 !Molecular energy (not used)   
2.6962 !Valency angle conjugation parameter   
7 ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#   
alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.   
cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.   
ov/un;val1;n.u.;val3,vval4   
C 1.3825 4.0000 12.0000 1.9133 0.1853 0.9000 1.1359 4.0000   
9.7602 2.1346 4.0000 33.2433 79.5548 5.8678 7.0000 0.0000   
1.2104 0.0000 199.0303 8.6991 34.7289 13.3894 0.8563 0.0000   
-2.8983 2.5000 1.0564 4.0000 2.9663 0.0000 0.0000 0.0000   
H 0.7853 1.0000 1.0080 1.5904 0.0419 1.0206 -0.1000 1.0000   
9.3557 5.0518 1.0000 0.0000 121.1250 5.3200 7.4366 1.0000   
-0.1000 0.0000 62.4879 1.9771 3.3517 0.7571 1.0698 0.0000   
-15.7683 2.1488 1.0338 1.0000 2.8793 0.0000 0.0000 0.0000   
O 1.2477 2.0000 15.9990 1.9236 0.0904 1.0503 1.0863 6.0000   
10.2127 7.7719 4.0000 36.9573 116.0768 8.5000 8.9989 2.0000   
0.9088 1.0003 60.8726 20.4140 3.3754 0.2702 0.9745 0.0000   
-3.6141 2.7025 1.0493 4.0000 2.9225 0.0000 0.0000 0.0000   
N 1.2333 3.0000 14.0000 1.9324 0.1376 0.8596 1.1748 5.0000   
10.0667 7.8431 4.0000 32.2482 100.0000 6.8418 6.3404 2.0000   
1.0433 13.7673 119.9837 2.1961 3.0696 2.7683 0.9745 0.0000

-4.3875 2.6192 1.0183 4.0000 2.8793 0.0000 0.0000 0.0000   
S 1.9401 2.0000 32.0600 2.0629 0.2095 1.0316 1.5483 6.0000   
9.9553 4.9055 4.0000 52.9998 112.1416 6.5181 8.2345 2.0000   
1.4601 9.6977 71.1843 5.7487 23.2859 12.7147 0.9745 0.0000   
-11.0200 2.7266 1.0338 6.2998 2.8793 0.0000 0.0000 0.0000   
Si 2.0291 4.0000 28.0600 2.0043 0.1247 0.8218 1.5023 4.0000   
13.0000 2.0618 4.0000 11.8211 136.4845 1.8038 7.3852 0.0000   
-1.0000 0.0000 126.5182 3.6038 8.5961 0.2368 0.8563 0.0000   
-3.5163 4.2105 1.0338 6.2998 2.5791 0.0000 0.0000 0.0000   
X -0.1000 2.0000 1.0080 2.0000 0.0000 1.0000 -0.1000 6.0000   
10.0000 2.5000 4.0000 0.0000 0.0000 8.5000 15.0000 0.0000   
-0.1000 0.0000 127.6226 8.7410 13.3640 0.6690 0.9745 0.0000   
-11.0000 2.7466 1.0338 6.2998 2.8793 0.0000 0.0000 0.0000   
19 ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6   
pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr   
1 1 156.5953 100.0397 80.0000 -0.8157 -0.4591 1.0000 37.7369 0.4235   
0.4527 -0.1000 9.2605 1.0000 -0.0750 6.8316 1.0000 0.0000   
1 2 170.2316 0.0000 0.0000 -0.5931 0.0000 1.0000 6.0000 0.7140   
5.2267 1.0000 0.0000 1.0000 -0.0500 6.8315 0.0000 0.0000   
2 2 156.0973 0.0000 0.0000 -0.1377 0.0000 1.0000 6.0000 0.8240   
2.9907 1.0000 0.0000 1.0000 -0.0593 4.8358 0.0000 0.0000   
1 3 160.4802 105.1693 23.3059 -0.3873 -0.1613 1.0000 10.8851 1.0000   
0.5341 -0.3174 7.0303 1.0000 -0.1463 5.2913 0.0000 0.0000   
3 3 60.1463 176.6202 51.1430 -0.2802 -0.1244 1.0000 29.6439 0.9114   
0.2441 -0.1239 7.6487 1.0000 -0.1302 6.2919 1.0000 0.0000   
1 4 134.1215 140.2179 79.9745 0.0163 -0.1428 1.0000 27.0617 0.2000   
0.1387 -0.3681 7.1611 1.0000 -0.1000 5.0825 1.0000 0.0000   
3 4 130.8596 169.4551 40.0000 0.3837 -0.1639 1.0000 35.0000 0.2000   
1.0000 -0.3579 7.0004 1.0000 -0.1193 6.8773 1.0000 0.0000   
4 4 157.9384 82.5526 152.5336 0.4010 -0.1034 1.0000 12.4261 0.5828   
0.1578 -0.1509 11.9186 1.0000 -0.0861 5.4271 1.0000 0.0000   
2 3 180.4373 0.0000 0.0000 -0.8074 0.0000 1.0000 6.0000 0.5514   
1.2490 1.0000 0.0000 1.0000 -0.0657 5.0451 0.0000 0.0000   
2 4 231.8173 0.0000 0.0000 -0.3364 0.0000 1.0000 6.0000 0.4402   
8.8910 1.0000 0.0000 1.0000 -0.0327 6.5754 0.0000 0.0000   
1 5 129.1942 74.3656 55.2528 0.1066 -0.5211 1.0000 18.9617 0.5950   
0.2950 -0.2398 8.0314 1.0000 -0.1019 5.6754 1.0000 0.0000   
2 5 151.3159 0.0000 0.0000 -0.4644 0.0000 1.0000 6.0000 0.5950   
9.4365 1.0000 0.0000 1.0000 -0.0303 7.0100 1.0000 0.0000   
3 5 0.0000 0.0000 0.0000 0.5563 -0.4038 1.0000 49.5611 0.6000   
0.4259 -0.4577 12.7569 1.0000 -0.1100 7.1145 1.0000 0.0000   
4 5 0.0000 0.0000 0.0000 0.4438 -0.2034 1.0000 40.3399 0.6000   
0.3296 -0.3153 9.1227 1.0000 -0.1805 5.6864 1.0000 0.0000   
5 5 96.1871 93.7006 68.6860 0.0955 -0.4781 1.0000 17.8574 0.6000   
0.2723 -0.2373 9.7875 1.0000 -0.0950 6.4757 1.0000 0.0000   
1 6 90.6281 6.3660 0.0000 0.3176 -0.5558 1.0000 17.2117 0.5577   
0.7223 -0.2118 7.7440 1.0000 -0.1039 5.4442 1.0000 0.0000   
2 6 137.1002 0.0000 0.0000 -0.1902 0.0000 1.0000 6.0000 0.4256   
17.7186 1.0000 0.0000 1.0000 -0.0377 6.4281 0.0000 0.0000   
3 6 230.7615 93.6959 43.3991 -0.3617 -0.3000 1.0000 36.0000 0.3161   
0.9856 -0.3882 4.6686 1.0000 -0.3960 4.5499 1.0000 0.0000   
6 6 72.8867 50.0318 30.0000 0.9983 -0.3000 1.0000 16.0000 0.1000   
1.0538 -0.0447 10.6176 1.0000 -0.1452 8.0404 0.0000 0.0000   
11 ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2   
1 2 0.1219 1.4000 9.8442 1.1203 -1.0000 -1.0000   
2 3 0.0344 1.6800 10.3247 0.9013 -1.0000 -1.0000   
2 4 0.1059 1.8290 9.7818 0.9598 -1.0000 -1.0000   
1 3 0.1131 1.8523 9.8442 1.2775 1.1342 1.0621   
1 4 0.1447 1.8766 9.7990 1.3436 1.1885 1.1363   
3 4 0.1048 2.0003 10.1220 1.3173 1.1096 1.0206

1 5 0.1997 2.0109 9.8603 1.6611 1.3423 -1.0000   
2 5 0.0938 1.8133 9.6519 1.3629 -1.0000 -1.0000   
1 6 0.0250 1.7695 12.4753 1.5866 1.4409 -1.0000   
2 6 0.0291 1.6805 12.5137 1.3429 -1.0000 -1.0000   
3 6 0.1958 1.7958 11.1207 1.6105 1.1632 -1.0000   
71 ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2   
1 1 1 67.2326 22.0695 1.6286 0.0000 1.7959 15.4141 1.8089   
1 1 2 65.2527 14.3185 6.2977 0.0000 0.5645 0.0000 1.1530   
2 1 2 70.0840 25.3540 3.4508 0.0000 0.0050 0.0000 3.0000   
1 2 2 0.0000 0.0000 6.0000 0.0000 0.0000 0.0000 1.0400   
1 2 1 0.0000 3.4110 7.7350 0.0000 0.0000 0.0000 1.0400   
2 2 2 0.0000 27.9213 5.8635 0.0000 0.0000 0.0000 1.0400   
1 1 3 49.5561 7.3771 4.9568 0.0000 0.7533 15.9906 1.0010   
3 1 3 77.1171 39.8746 2.5403 -24.3902 1.7740 -42.9758 2.1240   
1 1 4 66.1305 12.4661 7.0000 0.0000 3.0000 50.0000 1.1880   
3 1 4 73.9544 12.4661 7.0000 0.0000 3.0000 0.0000 1.1880   
4 1 4 64.1581 12.4661 7.0000 0.0000 3.0000 0.0000 1.1880   
2 1 3 65.0000 14.2057 4.8649 0.0000 0.3504 0.0000 1.7185   
2 1 4 74.2929 31.0883 2.6184 0.0000 0.0755 0.0000 1.0500   
1 2 4 0.0000 0.0019 6.3000 0.0000 0.0000 0.0000 1.0400   
1 3 1 74.3994 44.7500 0.7982 0.0000 3.0000 0.0000 1.0528   
1 3 3 77.9854 36.6201 2.0201 0.0000 0.7434 67.0264 3.0000   
1 3 4 82.4890 31.4554 0.9953 0.0000 1.6310 0.0000 1.0783   
3 3 3 80.7324 30.4554 0.9953 0.0000 1.6310 50.0000 1.0783   
3 3 4 84.3637 31.4554 0.9953 0.0000 1.6310 0.0000 1.0783   
4 3 4 89.7071 31.4554 0.9953 0.0000 1.6310 0.0000 1.1519   
1 3 2 71.5018 21.7062 0.4735 0.0000 0.5186 0.0000 1.1793   
2 3 3 84.9468 23.3540 1.5057 0.0000 2.6374 0.0000 1.3023   
2 3 4 75.6201 18.7919 0.9833 0.0000 0.1218 0.0000 1.0500   
2 3 2 77.0645 10.4737 1.2895 0.0000 0.9924 0.0000 1.1043   
1 4 1 66.0330 22.0295 1.4442 0.0000 1.6777 0.0000 1.0500   
1 4 3 103.3204 33.0381 0.5787 0.0000 1.6777 0.0000 1.0500   
1 4 4 104.1335 8.6043 1.6495 0.0000 1.6777 0.0000 1.0500   
3 4 3 74.1978 42.1786 1.7845 -18.0069 1.6777 0.0000 1.0500   
3 4 4 74.8600 43.7354 1.1572 -0.9193 1.6777 0.0000 1.0500   
4 4 4 75.0538 14.8267 5.2794 0.0000 1.6777 0.0000 1.0500   
1 4 2 69.1106 25.5067 1.1003 0.0000 0.0222 0.0000 1.0369   
2 4 3 81.3686 40.0712 2.2396 0.0000 0.0222 0.0000 1.0369   
2 4 4 83.0104 43.4766 1.5328 0.0000 0.0222 0.0000 1.0500   
2 4 2 70.8687 12.0168 5.0132 0.0000 0.0222 0.0000 1.1243   
1 2 3 0.0000 25.0000 3.0000 0.0000 1.0000 0.0000 1.0400   
1 2 4 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400   
1 2 5 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400   
3 2 3 0.0000 0.0148 6.0000 0.0000 0.0000 0.0000 1.0400   
3 2 4 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400   
4 2 4 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400   
2 2 3 0.0000 9.7025 6.0000 0.0000 0.0000 0.0000 1.0400   
2 2 4 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400   
1 1 5 73.9923 24.7559 1.8287 0.1463 0.0059 0.0000 1.0600   
1 5 1 86.7521 36.5756 2.0199 0.1463 0.0058 0.0000 1.0600   
2 1 5 75.1310 24.8619 1.8104 0.0000 0.0050 0.0000 1.0600   
1 5 2 85.3326 36.9451 2.1403 0.0000 0.0388 0.0000 1.0706   
1 5 5 86.0081 37.0451 2.1403 0.1463 0.1070 0.0000 1.0098   
2 5 2 92.9959 36.9602 2.0403 0.0000 0.0050 0.0000 1.0200   
2 5 5 83.2918 36.9451 2.0199 0.0000 0.0050 0.0000 1.0600   
2 2 5 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400   
6 6 6 71.6771 13.0081 3.6376 0.0000 0.2384 0.0000 1.3185   
2 6 6 89.1207 11.7566 1.1579 0.0000 0.0100 0.0000 1.2975   
2 6 2 26.3763 5.5393 0.9656 0.0000 2.3381 0.0000 1.1704   
3 6 6 85.6335 17.1826 6.5759 0.0000 0.4105 0.0000 1.6398

2 6 3 59.6558 6.8748 7.0452 0.0000 4.0000 0.0000 1.0400   
3 6 3 72.7359 17.5203 2.4434 0.0000 0.0100 0.0000 1.7374   
6 3 6 18.3653 5.7702 3.4915 0.0000 4.0000 0.0000 1.9438   
2 3 6 57.5894 40.0000 8.0000 0.0000 3.8263 0.0000 1.0534   
3 3 6 54.5893 38.8349 7.6245 0.0000 2.7656 0.0000 3.0000   
2 2 6 0.0000 47.1300 6.0000 0.0000 1.6371 0.0000 1.0400   
6 2 6 0.0000 31.5209 6.0000 0.0000 1.6371 0.0000 1.0400   
3 2 6 0.0000 31.0427 4.5625 0.0000 1.6371 0.0000 1.0400   
1 1 6 63.8858 35.1811 0.6236 0.0000 2.6344 0.0000 2.3890   
1 6 1 71.6429 31.1160 0.5107 0.0000 0.0100 0.0000 1.9113   
6 1 6 63.2523 33.3810 2.2952 0.0000 0.0201 0.0000 1.7191   
1 6 6 70.9876 29.7098 1.0210 0.0000 0.0100 0.0000 1.8242   
2 1 6 96.9319 10.9008 1.4627 0.0000 2.4557 0.0000 1.5109   
1 6 2 73.9320 16.6559 3.0433 0.0000 0.7961 0.0000 1.4005   
1 3 6 91.5678 5.9243 2.4284 0.0000 2.9840 0.0000 1.0400   
1 6 3 96.3796 36.5757 0.8505 0.0000 3.6964 0.0000 1.6527   
3 1 6 42.5553 40.0000 1.5855 0.0000 1.0802 0.0000 1.1584   
34 ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n   
1 1 1 1 -0.2500 11.5822 0.1879 -4.7057 -2.2047 0.0000 0.0000   
1 1 1 2 -0.2500 31.2596 0.1709 -4.6391 -1.9002 0.0000 0.0000   
2 1 1 2 -0.1770 30.0252 0.4340 -5.0019 -2.0697 0.0000 0.0000   
1 1 1 3 -0.7098 22.2951 0.0060 -2.5000 -2.1688 0.0000 0.0000   
2 1 1 3 -0.3568 22.6472 0.6045 -4.0088 -1.0000 0.0000 0.0000   
3 1 1 3 -0.0528 6.8150 0.7498 -5.0913 -1.0000 0.0000 0.0000   
1 1 3 1 2.0007 25.5641 -0.0608 -2.6456 -1.1766 0.0000 0.0000   
1 1 3 2 -1.1953 42.1545 -1.0000 -8.0821 -1.0000 0.0000 0.0000   
2 1 3 1 -0.9284 34.3952 0.7285 -2.5440 -2.4641 0.0000 0.0000   
2 1 3 2 -2.5000 79.6980 1.0000 -3.5697 -2.7501 0.0000 0.0000   
1 1 3 3 -0.0179 5.0603 -0.1894 -2.5000 -2.0399 0.0000 0.0000   
2 1 3 3 -0.5583 80.0000 1.0000 -4.4000 -3.0000 0.0000 0.0000   
3 1 3 1 -2.5000 76.0427 -0.0141 -3.7586 -2.9000 0.0000 0.0000   
3 1 3 2 0.0345 78.9586 -0.6810 -4.1777 -3.0000 0.0000 0.0000   
3 1 3 3 -2.5000 66.3525 0.3986 -3.0293 -3.0000 0.0000 0.0000   
1 3 3 1 2.5000 -0.5332 1.0000 -3.5096 -2.9000 0.0000 0.0000   
1 3 3 2 -2.5000 3.3219 0.7180 -5.2021 -2.9330 0.0000 0.0000   
2 3 3 2 2.2500 -6.2288 1.0000 -2.6189 -1.0000 0.0000 0.0000   
1 3 3 3 0.0531 -17.3983 1.0000 -2.5000 -2.1584 0.0000 0.0000   
2 3 3 3 0.4723 -12.4144 -1.0000 -2.5000 -1.0000 0.0000 0.0000   
3 3 3 3 -2.5000 -25.0000 1.0000 -2.5000 -1.0000 0.0000 0.0000   
0 1 2 0 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000   
0 2 2 0 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000   
0 2 3 0 0.0000 0.1000 0.0200 -2.5415 0.0000 0.0000 0.0000   
0 1 1 0 0.0000 50.0000 0.3000 -4.0000 -2.0000 0.0000 0.0000   
0 3 3 0 0.5511 25.4150 1.1330 -5.1903 -1.0000 0.0000 0.0000   
0 1 4 0 -2.4242 128.1636 0.3739 -6.6098 -2.0000 0.0000 0.0000   
0 2 4 0 0.0000 0.1000 0.0200 -2.5415 0.0000 0.0000 0.0000   
0 3 4 0 1.4816 55.6641 0.0004 -7.0465 -2.7831 0.0000 0.0000   
0 4 4 0 -0.3244 27.7086 0.0039 -2.8272 -2.0000 0.0000 0.0000   
4 1 4 4 -5.5181 8.9706 0.0004 -6.1782 -2.0000 0.0000 0.0000   
0 1 5 0 0.1515 29.0501 0.0792 -4.5064 -1.0200 0.0000 0.0000   
0 5 5 0 -0.0054 0.1000 0.1715 -2.2256 -1.0000 0.0000 0.0000   
0 2 5 0 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000   
0 ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1   
3 2 3 1.9682 -4.4628 1.7976 3.0000   
3 2 4 2.0000 -6.0000 1.7976 3.0000   
4 2 3 1.2000 -2.0000 1.7976 3.0000   
4 2 4 1.2979 -6.0000 1.7976 3.0000   
3 2 5 1.5000 -2.0000 1.7976 3.0000   
4 2 5 1.5000 -2.0000 1.7976 3.0000   
5 2 3 1.5000 -2.0000 1.7976 3.0000

5 2 4 1.5000 -2.0000 1.7976 3.0000   
5 2 5 1.5000 -2.0000 1.7976 3.0000