

Electronic Supplementary Information

Influence of carbon concentration on the electronic structure and magnetic properties of carbon implanted ZnO thin films

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The contribution of each atom in the unit cell of C incorporated ZnO to the total magnetic moment:

C in Interstitial Position

O 34 :MMI070: MAGNETIC MOMENT IN SPHERE 70 = 0.00000 MULT= 1 <-- C 2nd Neighbour
O 25 :MMI061: MAGNETIC MOMENT IN SPHERE 61 = 0.00001 MULT= 1 <-- C 2nd Neighbour
Zn 25 :MMI025: MAGNETIC MOMENT IN SPHERE 25 = 0.00023 MULT= 1
Zn 35 :MMI035: MAGNETIC MOMENT IN SPHERE 35 = 0.00028 MULT= 1 <-- C 2nd Neighbour
Zn 3 :MMI003: MAGNETIC MOMENT IN SPHERE 3 = 0.00028 MULT= 1 <-- C 2nd Neighbour
Zn 14 :MMI014: MAGNETIC MOMENT IN SPHERE 14 = 0.00029 MULT= 1
Zn 16 :MMI016: MAGNETIC MOMENT IN SPHERE 16 = 0.00029 MULT= 1
Zn 18 :MMI018: MAGNETIC MOMENT IN SPHERE 18 = 0.00029 MULT= 1
Zn 8 :MMI008: MAGNETIC MOMENT IN SPHERE 8 = 0.00029 MULT= 1
Zn 2 :MMI002: MAGNETIC MOMENT IN SPHERE 2 = 0.00030 MULT= 1 <-- C 2nd Neighbour
Zn 15 :MMI015: MAGNETIC MOMENT IN SPHERE 15 = 0.00032 MULT= 1
O 26 :MMI062: MAGNETIC MOMENT IN SPHERE 62 = 0.00033 MULT= 1 <-- C 2nd Neighbour
Zn 10 :MMI010: MAGNETIC MOMENT IN SPHERE 10 = 0.00033 MULT= 1

Zn 17 :MMI017: MAGNETIC MOMENT IN SPHERE 17 = 0.00033 MULT= 1
Zn 34 :MMI034: MAGNETIC MOMENT IN SPHERE 34 = 0.00033 MULT= 1 <-- C 2nd Neighbour
Zn 1 :MMI001: MAGNETIC MOMENT IN SPHERE 1 = 0.00034 MULT= 1 <-- C 2nd Neighbour
Zn 26 :MMI026: MAGNETIC MOMENT IN SPHERE 26 = 0.00036 MULT= 1 <-- C 2nd Neighbour
Zn 33 :MMI033: MAGNETIC MOMENT IN SPHERE 33 = 0.00036 MULT= 1 <-- C 2nd Neighbour
Zn 9 :MMI009: MAGNETIC MOMENT IN SPHERE 9 = 0.00039 MULT= 1
Zn 5 :MMI005: MAGNETIC MOMENT IN SPHERE 5 = 0.00040 MULT= 1
Zn 11 :MMI011: MAGNETIC MOMENT IN SPHERE 11 = 0.00048 MULT= 1 <-- C 2nd Neighbour
Zn 7 :MMI007: MAGNETIC MOMENT IN SPHERE 7 = 0.00050 MULT= 1
Zn 6 :MMI006: MAGNETIC MOMENT IN SPHERE 6 = 0.00051 MULT= 1
Zn 36 :MMI036: MAGNETIC MOMENT IN SPHERE 36 = 0.00053 MULT= 1 <-- C 2nd Neighbour
O 16 :MMI052: MAGNETIC MOMENT IN SPHERE 52 = 0.00072 MULT= 1 <-- C 2nd Neighbour
Zn 13 :MMI013: MAGNETIC MOMENT IN SPHERE 13 = 0.00073 MULT= 1
Zn 28 :MMI028: MAGNETIC MOMENT IN SPHERE 28 = 0.00077 MULT= 1 <-- C 2nd Neighbour
O 17 :MMI053: MAGNETIC MOMENT IN SPHERE 53 = 0.00081 MULT= 1
O 15 :MMI051: MAGNETIC MOMENT IN SPHERE 51 = 0.00082 MULT= 1
O 28 :MMI064: MAGNETIC MOMENT IN SPHERE 64 = 0.00082 MULT= 1 <-- C 2nd Neighbour
O 13 :MMI049: MAGNETIC MOMENT IN SPHERE 49 = 0.00083 MULT= 1
O 32 :MMI068: MAGNETIC MOMENT IN SPHERE 68 = 0.00090 MULT= 1
O 30 :MMI066: MAGNETIC MOMENT IN SPHERE 66 = 0.00099 MULT= 1
O 36 :MMI072: MAGNETIC MOMENT IN SPHERE 72 = 0.00099 MULT= 1
O 5 :MMI041: MAGNETIC MOMENT IN SPHERE 41 = 0.00102 MULT= 1
O 1 :MMI037: MAGNETIC MOMENT IN SPHERE 37 = 0.00114 MULT= 1
O 29 :MMI065: MAGNETIC MOMENT IN SPHERE 65 = 0.00125 MULT= 1 <-- C 2nd Neighbour
O 31 :MMI067: MAGNETIC MOMENT IN SPHERE 67 = 0.00142 MULT= 1 <-- C 2nd Neighbour

O 3 :MMI039: MAGNETIC MOMENT IN SPHERE 39 = 0.00153 MULT= 1
O 6 :MMI042: MAGNETIC MOMENT IN SPHERE 42 = 0.00158 MULT= 1 <-- C 2nd Neighbour
O 20 :MMI056: MAGNETIC MOMENT IN SPHERE 56 = 0.00161 MULT= 1 <-- C 2nd Neighbour
O 22 :MMI058: MAGNETIC MOMENT IN SPHERE 58 = 0.00169 MULT= 1
Zn 24 :MMI024: MAGNETIC MOMENT IN SPHERE 24 = 0.00176 MULT= 1 <-- C 2nd Neighbour
Zn 4 :MMI004: MAGNETIC MOMENT IN SPHERE 4 = 0.00177 MULT= 1 <-- C 2nd Neighbour
O 9 :MMI045: MAGNETIC MOMENT IN SPHERE 45 = 0.00181 MULT= 1 <-- C 2nd Neighbour
O 14 :MMI050: MAGNETIC MOMENT IN SPHERE 50 = 0.00184 MULT= 1
O 4 :MMI040: MAGNETIC MOMENT IN SPHERE 40 = 0.00184 MULT= 1 <-- C 2nd Neighbour
Zn 31 :MMI031: MAGNETIC MOMENT IN SPHERE 31 = 0.00187 MULT= 1 <-- C 2nd Neighbour
O 18 :MMI054: MAGNETIC MOMENT IN SPHERE 54 = 0.00191 MULT= 1
O 24 :MMI060: MAGNETIC MOMENT IN SPHERE 60 = 0.00218 MULT= 1
O 7 :MMI043: MAGNETIC MOMENT IN SPHERE 43 = 0.00219 MULT= 1
Zn 12 :MMI012: MAGNETIC MOMENT IN SPHERE 12 = 0.00285 MULT= 1 <-- C 2nd Neighbour
O 12 :MMI048: MAGNETIC MOMENT IN SPHERE 48 = 0.00319 MULT= 1
O 11 :MMI047: MAGNETIC MOMENT IN SPHERE 47 = 0.00321 MULT= 1
Zn 32 :MMI032: MAGNETIC MOMENT IN SPHERE 32 = 0.00331 MULT= 1 <-- C 2nd Neighbour
O 35 :MMI071: MAGNETIC MOMENT IN SPHERE 71 = 0.00424 MULT= 1 <-- C 2nd Neighbour
O 23 :MMI059: MAGNETIC MOMENT IN SPHERE 59 = 0.00468 MULT= 1 <-- C 2nd Neighbour
Zn 20 :MMI020: MAGNETIC MOMENT IN SPHERE 20 = 0.00582 MULT= 1 <-- C 1st Neighbour
O 33 :MMI069: MAGNETIC MOMENT IN SPHERE 69 = 0.00588 MULT= 1 <-- C 2nd Neighbour
Zn 21 :MMI021: MAGNETIC MOMENT IN SPHERE 21 = 0.00595 MULT= 1 <-- C 1st Neighbour
Zn 19 :MMI019: MAGNETIC MOMENT IN SPHERE 19 = 0.00636 MULT= 1 <-- C 1st Neighbour
O 2 :MMI038: MAGNETIC MOMENT IN SPHERE 38 = 0.00668 MULT= 1 <-- C 2nd Neighbour
Zn 27 :MMI027: MAGNETIC MOMENT IN SPHERE 27 = 0.00779 MULT= 1 <-- C 2nd Neighbour

Zn 23 :MMI023: MAGNETIC MOMENT IN SPHERE 23 = 0.00858 MULT= 1 <-- C 2nd Neighbour
Zn 22 :MMI022: MAGNETIC MOMENT IN SPHERE 22 = 0.02012 MULT= 1 <-- C 1st Neighbour
Zn 29 :MMI029: MAGNETIC MOMENT IN SPHERE 29 = 0.03132 MULT= 1 <-- C 1st Neighbour
O 8 :MMI044: MAGNETIC MOMENT IN SPHERE 44 = 0.03392 MULT= 1 <-- C 1st Neighbour
Zn 30 :MMI030: MAGNETIC MOMENT IN SPHERE 30 = 0.03509 MULT= 1 <-- C 1st Neighbour
O 10 :MMI046: MAGNETIC MOMENT IN SPHERE 46 = 0.04719 MULT= 1 <-- C 1st Neighbour
O 19 :MMI055: MAGNETIC MOMENT IN SPHERE 55 = 0.08185 MULT= 1 <-- C 1st Neighbour
O 21 :MMI057: MAGNETIC MOMENT IN SPHERE 57 = 0.11229 MULT= 1 <-- C 1st Neighbour
O 27 :MMI063: MAGNETIC MOMENT IN SPHERE 63 = 0.19032 MULT= 1 <-- C 1st Neighbour
C 1 :MMI073: MAGNETIC MOMENT IN SPHERE 73 = 0.60413 MULT= 1
Free e :MMINT: MAGNETIC MOMENT IN THE INTERST. = 0.61438
Total :MMTOT: SPIN MAGNETIC MOMENT IN THE CELL = 1.88372

Carbon Neighbourhood (0-3 Å)

I(C1-Zn19) = 2.55024(0) Å

I(C1-Zn20) = 2.54576(0) Å

I(C1-Zn21) = 2.45566(0) Å

I(C1-Zn22) = 2.23497(0) Å

I(C1-Zn29) = 2.14926(0) Å

I(C1-Zn30) = 2.10019(0) Å

I(C1- O8) = 2.79078(0) Å

I(C1- O10) = 2.70019(0) Å

I(C1- O19) = 2.43402(0) Å

I(C1- O21) = 2.28259(0) Å

I(C1- O27) = 1.64309(0) Å

Average bond length = 2.3533 Å

Polyhedral volume = 25.9619 Å³

Carbon Neighbourhood (3-5 Å)

I(C1-Zn1) = 4.37903(0) Å

I(C1-Zn2) = 4.61380(0) Å

I(C1-Zn3) = 4.30578(0) Å

I(C1-Zn4) = 4.43144(0) Å

I(C1-Zn11) = 4.09994(0) Å

I(C1-Zn12) = 4.37064(0) Å

I(C1-Zn23) = 4.13723(0) Å

I(C1-Zn24) = 3.95417(0) Å

I(C1-Zn26) = 4.91612(0) Å

I(C1-Zn27) = 4.30816(0) Å

I(C1-Zn28) = 4.36721(0) Å

I(C1-Zn31) = 3.79515(0) Å

I(C1-Zn32) = 3.68522(0) Å

I(C1-Zn33) = 4.95975(0) Å

I(C1-Zn34) = 4.87155(0) Å

I(C1-Zn35) = 4.80901(0) Å

I(C1-Zn36) = 4.78670(0) Å

I(C1- O2) = 3.05852(0) Å

I(C1- O4) = 4.36974(0) Å

I(C1- O6) = 4.50543(0) Å

I(C1- O9) = 4.87497(0) Å

I(C1- O16) = 3.94205(0) Å

I(C1- O20) = 3.89937(0) Å

I(C1- O23) = 4.97412(0) Å

I(C1- O25) = 3.71612(0) Å

I(C1- O26) = 3.66221(0) Å

I(C1- O28) = 3.57538(0) Å

I(C1- O29) = 3.54056(0) Å

I(C1- O31) = 4.16303(0) Å

I(C1- O33) = 4.66065(0) Å

I(C1- O34) = 4.63942(0) Å

I(C1- O35) = 4.58582(0) Å

C in O Position

Zn 4 :MMI004: MAGNETIC MOMENT IN SPHERE 4 = 0.00003 MULT= 1

O 6 :MMI020: MAGNETIC MOMENT IN SPHERE 20 = -0.00005 MULT= 1

Zn 11 :MMI011: MAGNETIC MOMENT IN SPHERE 11 = 0.00014 MULT= 1

O 10 :MMI024: MAGNETIC MOMENT IN SPHERE 24 = 0.00015 MULT= 1

Zn 12 :MMI012: MAGNETIC MOMENT IN SPHERE 12 = 0.00016 MULT= 1

Zn 3 :MMI003: MAGNETIC MOMENT IN SPHERE 3 = 0.00016 MULT= 3

Zn 8 :MMI008: MAGNETIC MOMENT IN SPHERE 8 = 0.00022 MULT= 6 <-- C 2nd Neighbour

Zn 5 :MMI005: MAGNETIC MOMENT IN SPHERE 5 = 0.00023 MULT= 1

Zn 2 :MMI002: MAGNETIC MOMENT IN SPHERE 2 = 0.00024 MULT= 3

O 2 :MMI016: MAGNETIC MOMENT IN SPHERE 16 = 0.00026 MULT= 3 <-- C 2nd Neighbour

O 3 :MMI017: MAGNETIC MOMENT IN SPHERE 17 = 0.00035 MULT= 3 <-- C 2nd Neighbour

Zn 9 :MMI009: MAGNETIC MOMENT IN SPHERE 9 = 0.00038 MULT= 3 <-- C 2nd Neighbour

Zn 7 :MMI007: MAGNETIC MOMENT IN SPHERE 7 = 0.00043 MULT= 1 <-- C 2nd Neighbour

O 7 :MMI021: MAGNETIC MOMENT IN SPHERE 21 = 0.00091 MULT= 1
 O 4 :MMI018: MAGNETIC MOMENT IN SPHERE 18 = 0.00210 MULT= 3
 Zn 1 :MMI001: MAGNETIC MOMENT IN SPHERE 1 = 0.00217 MULT= 6 <-- C 2nd Neighbour
 O 13 :MMI027: MAGNETIC MOMENT IN SPHERE 27 = 0.00282 MULT= 1
 O 5 :MMI019: MAGNETIC MOMENT IN SPHERE 19 = 0.00312 MULT= 3
 Zn 6 :MMI006: MAGNETIC MOMENT IN SPHERE 6 = 0.00346 MULT= 3
 O 12 :MMI026: MAGNETIC MOMENT IN SPHERE 26 = 0.00350 MULT= 1
 O 1 :MMI015: MAGNETIC MOMENT IN SPHERE 15 = 0.00419 MULT= 6
 Zn 10 :MMI010: MAGNETIC MOMENT IN SPHERE 10 = 0.00606 MULT= 3
 O 11 :MMI025: MAGNETIC MOMENT IN SPHERE 25 = 0.03423 MULT= 6 <-- C 2nd Neighbour
 O 8 :MMI022: MAGNETIC MOMENT IN SPHERE 22 = 0.04058 MULT= 3 <-- C 2nd Neighbour
 O 9 :MMI023: MAGNETIC MOMENT IN SPHERE 23 = 0.04182 MULT= 3 <-- C 2nd Neighbour
 Zn 13 :MMI013: MAGNETIC MOMENT IN SPHERE 13 = 0.07618 MULT= 3 <-- C 1st Neighbour
 Zn 14 :MMI014: MAGNETIC MOMENT IN SPHERE 14 = 0.09231 MULT= 1 <-- C 1st Neighbour
 C 1 :MMI028: MAGNETIC MOMENT IN SPHERE 28 = 0.63353 MULT= 1
 Free e :MMINT: MAGNETIC MOMENT IN THE INTERST. = 0.49717
 Total :MMTOT: SPIN MAGNETIC MOMENT IN THE CELL = 2.00034

Carbon Neighbourhood (0-3 Å)

I(C1-Zn13) = 1.97465(0) Å

I(C1-Zn13) = 1.97465(0) Å

I(C1-Zn13) = 1.97465(0) Å

I(C1-Zn14) = 2.03309(0) Å

Average bond length = 1.9893 Å

Polyhedral volume = 4.0306 Å³

Carbon Neighbourhood (3-5 Å)

I(C1-Zn1) = 4.55783(0) Å

I(C1-Zn1) = 4.55783(0) Å

I(C1-Zn1) = 4.55783(0) Å

I(C1-Zn1) = 4.55783(0) Å

I(C1-Zn1) = 4.55783(0) Å

I(C1-Zn1) = 4.55783(0) Å

I(C1-Zn7) = 3.14873(0) Å

I(C1-Zn8) = 3.81941(0) Å

I(C1-Zn8) = 3.81941(0) Å

I(C1-Zn8) = 3.81941(0) Å

I(C1-Zn8) = 3.81941(0) Å

I(C1-Zn8) = 3.81941(0) Å

I(C1-Zn8) = 3.81941(0) Å

I(C1-Zn9) = 3.79058(0) Å

I(C1-Zn9) = 3.79058(0) Å

I(C1-Zn9) = 3.79058(0) Å

I(C1- O2) = 4.57893(0) Å

I(C1- O2) = 4.57893(0) Å

I(C1- O2) = 4.57893(0) Å

I(C1- O3) = 4.54737(0) Å

I(C1- O3) = 4.54737(0) Å

I(C1- O3) = 4.54737(0) Å

I(C1- O8) = 3.25034(0) Å

I(C1- O8) = 3.25034(0) Å

l(C1- O8) = 3.25034(0) Å

l(C1- O9) = 3.19378(0) Å

l(C1- O9) = 3.19378(0) Å

l(C1- O9) = 3.19378(0) Å

l(C1- O11) = 3.27137(0) Å

l(C1- O11) = 3.27136(0) Å

l(C1- O11) = 3.27137(0) Å

l(C1- O11) = 3.27137(0) Å

l(C1- O11) = 3.27137(0) Å

l(C1- O11) = 3.27137(0) Å

C in Zn Position

Zn 1 :MMI001: MAGNETIC MOMENT IN SPHERE 1 = 0.00000 MULT= 6

Zn 2 :MMI002: MAGNETIC MOMENT IN SPHERE 2 = 0.00000 MULT= 3

Zn 3 :MMI003: MAGNETIC MOMENT IN SPHERE 3 = 0.00000 MULT= 3

Zn 4 :MMI004: MAGNETIC MOMENT IN SPHERE 4 = 0.00000 MULT= 3

Zn 5 :MMI005: MAGNETIC MOMENT IN SPHERE 5 = 0.00000 MULT= 3

Zn 6 :MMI006: MAGNETIC MOMENT IN SPHERE 6 = 0.00000 MULT= 1

Zn 7 :MMI007: MAGNETIC MOMENT IN SPHERE 7 = 0.00000 MULT= 1

Zn 8 :MMI008: MAGNETIC MOMENT IN SPHERE 8 = 0.00000 MULT= 3

Zn 9 :MMI009: MAGNETIC MOMENT IN SPHERE 9 = 0.00000 MULT= 3

Zn 10 :MMI010: MAGNETIC MOMENT IN SPHERE 10 = 0.00000 MULT= 1

Zn 11 :MMI011: MAGNETIC MOMENT IN SPHERE 11 = 0.00000 MULT= 6

Zn 12 :MMI012: MAGNETIC MOMENT IN SPHERE 12 = 0.00000 MULT= 1

Zn 13 :MMI013: MAGNETIC MOMENT IN SPHERE 13 = 0.00000 MULT= 1

O 1 :MMI014: MAGNETIC MOMENT IN SPHERE 14 = 0.00000 MULT= 6
 O 2 :MMI015: MAGNETIC MOMENT IN SPHERE 15 = 0.00000 MULT= 3
 O 3 :MMI016: MAGNETIC MOMENT IN SPHERE 16 = 0.00000 MULT= 3
 O 4 :MMI017: MAGNETIC MOMENT IN SPHERE 17 = 0.00000 MULT= 1
 O 5 :MMI018: MAGNETIC MOMENT IN SPHERE 18 = 0.00000 MULT= 1
 O 6 :MMI019: MAGNETIC MOMENT IN SPHERE 19 = 0.00001 MULT= 3 <-- C 1st Neighbour
 O 7 :MMI020: MAGNETIC MOMENT IN SPHERE 20 = 0.00000 MULT= 1
 O 8 :MMI021: MAGNETIC MOMENT IN SPHERE 21 = 0.00000 MULT= 6
 O 9 :MMI022: MAGNETIC MOMENT IN SPHERE 22 = 0.00000 MULT= 3
 O 10 :MMI023: MAGNETIC MOMENT IN SPHERE 23 = 0.00000 MULT= 3
 O 11 :MMI024: MAGNETIC MOMENT IN SPHERE 24 = 0.00000 MULT= 1
 O 12 :MMI025: MAGNETIC MOMENT IN SPHERE 25 = 0.00000 MULT= 1
 O 13 :MMI026: MAGNETIC MOMENT IN SPHERE 26 = 0.00000 MULT= 3
 O 14 :MMI027: MAGNETIC MOMENT IN SPHERE 27 = 0.00003 MULT= 1 <-- C 1st Neighbour
 C 1 :MMI028: MAGNETIC MOMENT IN SPHERE 28 = 0.00005 MULT= 1
 Free e :MMINT: MAGNETIC MOMENT IN INTERSTITIAL = 0.00022
 Total :MMTOT: SPIN MAGNETIC MOMENT IN CELL = 0.00022

Carbon Neighbourhood

I(C1- O6) = 1.65929(0) Å

I(C1- O6) = 1.65929(0) Å

I(C1- O6) = 1.65929(0) Å

I(C1- O14) = 1.87864(0) Å

Average bond length = 1.7141 Å

Polyhedral volume = 2.5784 Å³