

Supporting information

Improved photocatalytic performance of double-walled TeSi

nanotubes: A hybrid density functional calculation

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Changji University, Changji 831100, China.

S1. The structural coordinates information of TeSi monolayer.

2

TeSi

SI 1.891144595210E+00 -1.091852841120E+00 7.712044867120E-01

TE 0.000000000000E+00 0.000000000000E+00 -7.712044867120E-01

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S2. The structural coordinates information of TeSi (30,30) single-walled nanotube

120

TeSi

SI	-2.192323844711E+00	1.915865441463E+01	0.000000000000E+00
SI	1.087470829289E+00	1.423765489133E+01	1.281964204548E+01
SI	1.087470829289E+00	1.423765489133E+01	-1.281964204548E+01
SI	-2.192323844711E+00	2.002624704244E+00	1.905370130113E+01
SI	-2.192323844711E+00	2.002624704244E+00	-1.905370130113E+01
SI	1.087470829289E+00	-1.126117451868E+01	1.549967701079E+01
SI	1.087470829279E+00	-1.126117451868E+01	-1.549967701079E+01
SI	-2.192323844711E+00	-1.873999184896E+01	3.983308233143E+00
SI	-2.192323844711E+00	-1.873999184896E+01	-3.983308233143E+00
SI	1.087470829279E+00	-1.659188142538E+01	-9.579327207313E+00
SI	1.087470829289E+00	-1.659188142538E+01	9.579327207313E+00
SI	-2.192323844711E+00	-5.920349803477E+00	-1.822096312447E+01
SI	-2.192323844711E+00	-5.920349803477E+00	1.822096312447E+01
SI	1.087470829289E+00	7.792526782458E+00	-1.750230171503E+01
SI	1.087470829279E+00	7.792526782458E+00	1.750230171503E+01
SI	-2.192323844711E+00	1.750230171503E+01	-7.792526782458E+00
SI	-2.192323844711E+00	1.750230171503E+01	7.792526782458E+00
SI	1.087470829289E+00	1.822096312447E+01	5.920349803477E+00
SI	1.087470829289E+00	1.822096312447E+01	-5.920349803477E+00

SI -2.192323844711E+00 9.579327207313E+00 1.659188142538E+01
SI -2.192323844711E+00 9.579327207313E+00 -1.659188142538E+01
SI 1.087470829279E+00 -3.983308233143E+00 1.873999184896E+01
SI 1.087470829289E+00 -3.983308233143E+00 -1.873999184896E+01
SI -2.192323844711E+00 -1.549967701079E+01 1.126117451868E+01
SI -2.192323844711E+00 -1.549967701079E+01 -1.126117451868E+01
SI 1.087470829279E+00 -1.905370130113E+01 -2.002624704244E+00
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SI 1.087470829289E+00 -8.211904681703E-15 -1.915865441463E+01
SI 1.087470829289E+00 -9.396892758052E-15 1.915865441463E+01
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SI 1.087470829289E+00 1.905370130113E+01 -2.002624704244E+00
SI 1.087470829279E+00 1.905370130113E+01 2.002624704244E+00
SI -2.192323844711E+00 1.549967701079E+01 1.126117451868E+01
SI -2.192323844711E+00 1.549967701079E+01 -1.126117451868E+01
SI 1.087470829289E+00 3.983308233143E+00 1.873999184896E+01
SI 1.087470829289E+00 3.983308233143E+00 -1.873999184896E+01
SI -2.192323844711E+00 -9.579327207313E+00 1.659188142538E+01
SI -2.192323844711E+00 -9.579327207313E+00 -1.659188142538E+01

SI 1.087470829279E+00 -1.822096312447E+01 5.920349803477E+00
SI 1.087470829289E+00 -1.822096312447E+01 -5.920349803477E+00
SI -2.192323844711E+00 -1.750230171503E+01 -7.792526782458E+00
SI -2.192323844711E+00 -1.750230171503E+01 7.792526782458E+00
SI 1.087470829289E+00 -7.792526782458E+00 -1.750230171503E+01
SI 1.087470829279E+00 -7.792526782458E+00 1.750230171503E+01
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SI -2.192323844711E+00 5.920349803477E+00 1.822096312447E+01
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SI 1.087470829289E+00 1.659188142538E+01 9.579327207313E+00
SI -2.192323844711E+00 1.873999184896E+01 3.983308233143E+00
SI -2.192323844711E+00 1.873999184896E+01 -3.983308233143E+00
SI 1.087470829289E+00 1.126117451868E+01 1.549967701079E+01
SI 1.087470829279E+00 1.126117451868E+01 -1.549967701079E+01
SI -2.192323844711E+00 -2.002624704244E+00 1.905370130113E+01
SI -2.192323844711E+00 -2.002624704244E+00 -1.905370130113E+01
SI 1.087470829289E+00 -1.423765489133E+01 1.281964204548E+01
SI 1.087470829289E+00 -1.423765489133E+01 -1.281964204548E+01
SI -2.192323844711E+00 -1.915865441463E+01 1.642380936339E-14
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TE 3.285588736049E+00 1.310681786155E+01 1.180143181042E+01
TE 3.285588736049E+00 1.310681786155E+01 -1.180143181042E+01

TE 5.794062049000E-03 1.843564649087E+00 1.754034596627E+01
TE 5.794062049000E-03 1.843564649087E+00 -1.754034596627E+01
TE 3.285588736049E+00 -1.036674680275E+01 1.426860287342E+01
TE 3.285588736039E+00 -1.036674680275E+01 -1.426860287342E+01
TE 5.794062049000E-03 -1.725155313610E+01 3.666930818080E+00
TE 5.794062049014E-03 -1.725155313610E+01 -3.666930818080E+00
TE 3.285588736039E+00 -1.527405808630E+01 -8.818481547749E+00
TE 3.285588736049E+00 -1.527405808630E+01 8.818481547749E+00
TE 5.794062048998E-03 -5.450121325674E+00 -1.677374867963E+01
TE 5.794062049004E-03 -5.450121325674E+00 1.677374867963E+01
TE 3.285588736049E+00 7.173599163518E+00 -1.611216752251E+01
TE 3.285588736039E+00 7.173599163518E+00 1.611216752251E+01
TE 5.794062049002E-03 1.611216752251E+01 -7.173599163518E+00
TE 5.794062048994E-03 1.611216752251E+01 7.173599163518E+00
TE 3.285588736049E+00 1.677374867963E+01 5.450121325674E+00
TE 3.285588736049E+00 1.677374867963E+01 -5.450121325674E+00
TE 5.794062049000E-03 8.818481547749E+00 1.527405808630E+01
TE 5.794062049009E-03 8.818481547749E+00 -1.527405808630E+01
TE 3.285588736039E+00 -3.666930818080E+00 1.725155313610E+01
TE 3.285588736049E+00 -3.666930818080E+00 -1.725155313610E+01
TE 5.794062048997E-03 -1.426860287342E+01 1.036674680275E+01
TE 5.794062048999E-03 -1.426860287342E+01 -1.036674680275E+01

TE 3.285588736039E+00 -1.754034596627E+01 -1.843564649087E+00

TE 3.285588736039E+00 -1.754034596627E+01 1.843564649087E+00

TE 5.794062049001E-03 -1.180143181042E+01 -1.310681786155E+01

TE 5.794062049013E-03 -1.180143181042E+01 1.310681786155E+01

TE 3.285588736049E+00 -7.559667640561E-15 -1.763696309550E+01

TE 3.285588736049E+00 -8.650537099285E-15 1.763696309550E+01

TE 5.794062048999E-03 1.180143181042E+01 -1.310681786155E+01

TE 5.794062049003E-03 1.180143181042E+01 1.310681786155E+01

TE 3.285588736049E+00 1.754034596627E+01 -1.843564649087E+00

TE 3.285588736039E+00 1.754034596627E+01 1.843564649087E+00

TE 5.794062049009E-03 1.426860287342E+01 1.036674680275E+01

TE 5.794062048993E-03 1.426860287342E+01 -1.036674680275E+01

TE 3.285588736049E+00 3.666930818080E+00 1.725155313610E+01

TE 3.285588736049E+00 3.666930818080E+00 -1.725155313610E+01

TE 5.794062049007E-03 -8.818481547749E+00 1.527405808630E+01

TE 5.794062049008E-03 -8.818481547749E+00 -1.527405808630E+01

TE 3.285588736039E+00 -1.677374867963E+01 5.450121325674E+00

TE 3.285588736049E+00 -1.677374867963E+01 -5.450121325674E+00

TE 5.794062049004E-03 -1.611216752251E+01 -7.173599163518E+00

TE 5.794062048998E-03 -1.611216752251E+01 7.173599163518E+00

TE 3.285588736049E+00 -7.173599163518E+00 -1.611216752251E+01

TE 3.285588736039E+00 -7.173599163518E+00 1.611216752251E+01

TE 5.794062049002E-03 5.450121325674E+00 -1.677374867963E+01
TE 5.794062049013E-03 5.450121325674E+00 1.677374867963E+01
TE 3.285588736049E+00 1.527405808630E+01 -8.818481547749E+00
TE 3.285588736049E+00 1.527405808630E+01 8.818481547749E+00
TE 5.794062049000E-03 1.725155313610E+01 3.666930818080E+00
TE 5.794062049003E-03 1.725155313610E+01 -3.666930818080E+00
TE 3.285588736049E+00 1.036674680275E+01 1.426860287342E+01
TE 3.285588736039E+00 1.036674680275E+01 -1.426860287342E+01
TE 5.794062049010E-03 -1.843564649087E+00 1.754034596627E+01
TE 5.794062049005E-03 -1.843564649087E+00 -1.754034596627E+01
TE 3.285588736049E+00 -1.310681786155E+01 1.180143181042E+01
TE 3.285588736049E+00 -1.310681786155E+01 -1.180143181042E+01
TE 5.794062049007E-03 -1.763696309550E+01 1.511933528110E-14

S3. The structural coordinates information of TeSi (15,15)@(30,30)double-walled nanotube

180

TeSi

SI	-2.110458497096E+00	1.016308361010E+01	0.000000000000E+00
SI	1.167905635583E+00	1.062289015266E+00	1.010700484695E+01
SI	1.167905635583E+00	1.062289015267E+00	-1.010700484695E+01
SI	-2.110458497096E+00	-9.940995849282E+00	2.113023897301E+00
SI	-2.110458497096E+00	-9.940995849282E+00	-2.113023897301E+00
SI	1.167905635583E+00	-3.140439918404E+00	-9.665280236351E+00
SI	1.167905635583E+00	-3.140439918401E+00	9.665280236354E+00
SI	-2.110458497096E+00	9.284438867657E+00	-4.133698510874E+00
SI	-2.110458497096E+00	9.284438867657E+00	4.133698510874E+00
SI	1.167905635583E+00	5.081338527602E+00	8.801136500262E+00
SI	1.167905635583E+00	5.081338527593E+00	-8.801136500259E+00
SI	-2.110458497096E+00	-8.222107355828E+00	5.973710663830E+00
SI	-2.110458497096E+00	-8.222107355828E+00	-5.973710663830E+00
SI	1.167905635583E+00	-6.800158260170E+00	-7.552340866569E+00
SI	1.167905635583E+00	-6.800158260169E+00	7.552340866570E+00
SI	-2.110458497096E+00	6.800430298506E+00	-7.552642995739E+00
SI	-2.110458497096E+00	6.800430298506E+00	7.552642995739E+00
SI	1.167905635583E+00	8.221778445996E+00	5.973471696858E+00

SI 1.167905635583E+00 8.221778445995E+00 -5.973471696857E+00
SI -2.110458497096E+00 -5.081541805052E+00 8.801488587131E+00
SI -2.110458497096E+00 -5.081541805052E+00 -8.801488587131E+00
SI 1.167905635583E+00 -9.284067461261E+00 -4.133533150094E+00
SI 1.167905635583E+00 -9.284067461263E+00 4.133533150096E+00
SI -2.110458497096E+00 3.140565550776E+00 -9.665666893040E+00
SI -2.110458497096E+00 3.140565550776E+00 9.665666893040E+00
SI 1.167905635583E+00 9.940598178573E+00 2.112939369781E+00
SI 1.167905635583E+00 9.940598178571E+00 -2.112939369785E+00
SI -2.110458497096E+00 -1.062331511828E+00 1.010740917470E+01
SI -2.110458497096E+00 -1.062331511828E+00 -1.010740917470E+01
SI 1.167905635583E+00 -1.016267705520E+01 -2.801980869549E-12
TE 9.915363827500E-02 8.662682025433E+00 0.000000000000E+00
TE 3.379076949291E+00 9.056725127821E-01 8.616898362772E+00
TE 3.379076949291E+00 9.056725127823E-01 -8.616898362774E+00
TE 9.915363827500E-02 -8.473381639099E+00 1.801072866926E+00
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TE 3.379076949291E+00 -2.677435303639E+00 -8.240298555854E+00
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TE 9.915363827499E-02 7.913753815340E+00 3.523430207059E+00
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TE 9.915363827500E-02 -7.008256975442E+00 5.091796739845E+00
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TE 3.379076949291E+00 -5.797590232316E+00 -6.438876267865E+00
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TE 9.915363827500E-02 5.796465676373E+00 -6.437627321953E+00
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TE 3.379076949291E+00 7.009616627594E+00 -5.092784584964E+00
TE 9.915363827500E-02 -4.331341012716E+00 7.502102698928E+00
TE 9.915363827500E-02 -4.331341012716E+00 -7.502102698928E+00
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TE 3.379076949291E+00 -7.915289140378E+00 3.524113777809E+00
TE 9.915363827500E-02 2.676915962726E+00 -8.238700188880E+00
TE 9.915363827500E-02 2.676915962726E+00 8.238700188880E+00
TE 3.379076949291E+00 8.475025535954E+00 1.801422287988E+00
TE 3.379076949291E+00 8.475025535952E+00 -1.801422287992E+00
TE 9.915363827500E-02 -9.054968398978E-01 8.615226946904E+00
TE 9.915363827500E-02 -9.054968398978E-01 -8.615226946904E+00
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SI 1.042879028429E+00 1.424312649101E+01 -1.282409604521E+01
SI -2.234575258020E+00 2.003376405938E+00 1.906085326507E+01
SI -2.234575258020E+00 2.003376405939E+00 -1.906085326507E+01
SI 1.042879028429E+00 -1.126560051216E+01 1.550517128948E+01
SI 1.042879028429E+00 -1.126560051216E+01 -1.550517128948E+01
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SI -2.234575258020E+00 -5.922572055604E+00 1.822780251327E+01
SI 1.042879028429E+00 7.795713732584E+00 -1.750859614633E+01
SI 1.042879028429E+00 7.795713732584E+00 1.750859614633E+01
SI -2.235682176033E+00 1.750931382648E+01 -7.795648775617E+00
SI -2.235682176033E+00 1.750931382648E+01 7.795648775617E+00
SI 1.042879028429E+00 1.822777328441E+01 5.922193234616E+00
SI 1.042879028429E+00 1.822777328441E+01 -5.922193234616E+00
SI -2.234575258020E+00 9.582922886792E+00 1.659810932493E+01
SI -2.234575258020E+00 9.582922886775E+00 -1.659810932493E+01
SI 1.042879028429E+00 -3.985116854910E+00 1.874681133601E+01
SI 1.042879028429E+00 -3.985116854910E+00 -1.874681133601E+01
SI -2.235682176033E+00 -1.550588679190E+01 1.126568618874E+01

SI -2.235682176033E+00 -1.550588679190E+01 -1.126568618874E+01

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SI -2.234575258020E+00 -1.282445400384E+01 1.424299911253E+01

SI 1.042879028429E+00 3.512479612215E-04 -1.916570091314E+01

SI 1.042879028429E+00 3.512479612215E-04 1.916570091314E+01

SI -2.235682176033E+00 1.282477809902E+01 -1.424335905667E+01

SI -2.235682176033E+00 1.282477809902E+01 1.424335905667E+01

SI 1.042879028429E+00 1.906067248279E+01 -2.003710587672E+00

SI 1.042879028429E+00 1.906067248279E+01 2.003710587672E+00

SI -2.234575258020E+00 1.550549494238E+01 1.126540149342E+01

SI -2.234575258020E+00 1.550549494238E+01 -1.126540149342E+01

SI 1.042879028429E+00 3.984429710210E+00 1.874695739312E+01

SI 1.042879028429E+00 3.984429710210E+00 -1.874695739312E+01

SI -2.235682176033E+00 -9.583165063100E+00 1.659852878660E+01

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