Supplementary Material

Electronic Structure of OsSi Calculated by MS-NEVPT2 with Inclusion of the Relativistic Effects

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1 Spectroscopic Parameters of the $\Lambda - S$ States of OsSi from MS-NEVPT2 with the DKH3 and X2C Hamiltonian

Table S1: Spectroscopic Parameters of the $\Lambda - \mathrm{S}$ States from MS-NEVPT2 with the DKH3 and X2C Hamiltonian[a]

	DKH3		X2C	
state	R_e (Å)	T_e (cm^{-1})	R_e (Å)	T_e (cm^{-1})
$X^3\Sigma^-$	2.115(0.001)	0(0)	2.115(0.001)	0(0)
$^3\Delta$(I)	2.079(0.001)	2146(131)	2.080(0.000)	2129(114)
$^1\Sigma^+$(I)	2.073(0.001)	5362(85)	2.073(0.001)	5351(74)
$^1\Gamma$	2.073(0.000)	7340(26)	2.073(0.000)	7337(23)
$^1\Delta$(I)	2.039(0.000)	11361(79)	2.031(0.008)	11389(107)
$^5\Pi$(I)	2.128(0.000)	12046(98)	2.128(0.000)	12046(98)
$^3\Phi$	2.152(0.000)	12553(52)	2.152(0.000)	12545(44)
$^3\Pi$(I)	2.152(0.000)	13601(55)	2.152(0.000)	13594(48)
$^3\Delta$(II)	2.051(0.002)	14766(88)	2.052(0.001)	14751(73)
$^3\Pi$(II)	2.189(0.000)	16107(98)	2.189(0.000)	16092(83)
$^1\Pi$(I)	2.142(0.000)	16077(59)	2.142(0.000)	16068(50)
$^5\Delta$(I)	2.227(0.000)	16937(84)	2.227(0.000)	16929(76)
$^5\Sigma^-$	2.126(0.009)	18767(92)	2.217(0.001)	18752(77)
$^1\Delta$(II)	2.102(0.000)	18882(51)	2.102(0.000)	18875(44)
$^1\Sigma^+$(II)	2.065(0.011)	19057(48)	2.073(0.003)	19205(100)
$^5\Delta$(II)	2.242(0.001)	19446(65)	2.242(0.001)	19435(54)
$^1\Phi$(I)	2.160(0.001)	19472(49)	2.160(0.001)	19465(42)
$^5\Pi$(II)	2.110(0.002)	20137(100)	2.110(0.002)	20122(85)
$^3\Pi$(III)	2.100(0.000)	20987(168)	2.100(0.000)	20963(144)
$^5\Gamma$	2.225(0.000)	21079(120)	2.225(0.000)	21061(102)
$^3\Sigma^+$(I)	2.112(0.005)	21621(69)	2.116(0.001)	21726(174)
$^1\Phi$(II)	2.104(0.001)	22669(122)	2.104(0.001)	22651(104)
$^1\Pi$(II)	2.116(0.000)	23019(186)	2.116(0.000)	22993(160)
$^5\Phi$	2.105(0.000)	23320(148)	2.105(0.000)	23299(127)
$^3\Delta$(III)	2.232(0.005)	24076(110)	2.238(0.001)	24048(82)
$^3\Sigma^+$(II)	2.248(0.004)	24301(67)	2.245(0.007)	24265(31)
$^5\Pi$(III)	2.118(0.002)	24466(142)	2.119(0.001)	24445(121)
$^7\Delta$	2.168(0.002)	25588(139)	2.168(0.002)	25567(118)

[a] Values in parentheses are the absolute errors of R_e and T_e respected to the DKH2 results.

2 Vertical Excitation Energies of Triplet States Calculated by TDDFT with the B3LYP Functional

Table S2: Comparing Vertical Excitation Energies of Triplet States Calculated by SA-TDDFT with the B3LYP Functional and the MS-NEVPT2, MS-CASPT2 Results[a]

States	$\Delta E(cm^{-1})^b$	f	$\Delta E(cm^{-1})^c$	f
$^3\Sigma^-$	0		0	
$^3\Delta$(I)	3067	0.0000	2134(3818)	0.0000
$^3\Phi$(I)	9622	0.0000	12043(13168)	0.0000
$^3\Pi$(I)	12330	0.0001	13221(14434)	0.0001
$^3\Delta$(II)	15167	0.0000	14434(16418)	0.0000
$^3\Pi$(II)	16213	0.0102	16585(18345)	0.0148
$^3\Pi$(III)	20687	0.0008	21407(23381)	0.0001
$^3\Sigma^+$(I)	22585	0.0088	22585(23579)	0.0017
$^3\Sigma^+$(II)	24007	0.0250	26079(26474)	0.0000
$^3\Pi$(IV)	24334	0.0000	22544(23382)	0.0000
$^3\Delta$(III)	24490	0.0000	25036(25738)	0.0000

[a] The bond length is chosen as 2.114 Å that is same as equilibrium bond length calculated by MS-NVEPT2.
[b] VEEs from SA-TDDFT.
[c] VEEs from MS-NEVPT2. The values in parenthesis are the MS-CASPT2 results.

3 The Number of States in Each Irrep on SA-CASSCF and MS-NEVPT2 Calculations

Table S3: Number of States on SA-CASSCF and MS-NEVPT2 Level under C_{2V} Symmetry

spin mul.	A_1	B_1	B_2	A_2
1	6	4	4	4
3	5	4	4	5
5	4	4	4	4
7	1	1	1	1

4 Potential Energy Curves of the $\Lambda - S$ States of OsSi Calculated by MS-NEVPT2

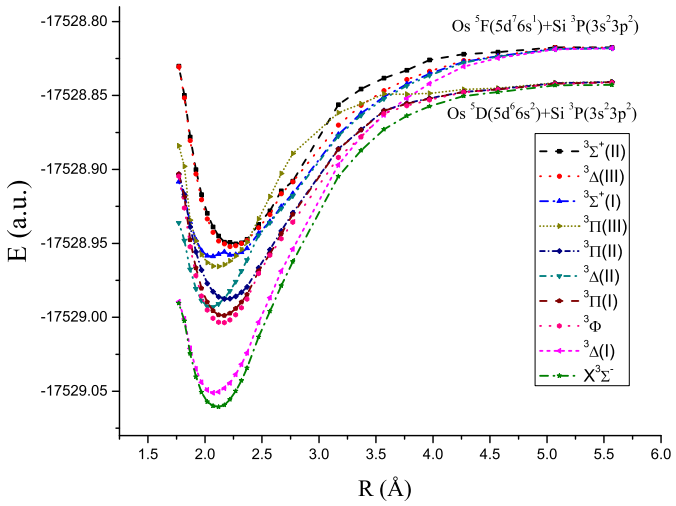

Figure S1: Potential Energy Curves of the Triplet States of OsSi.

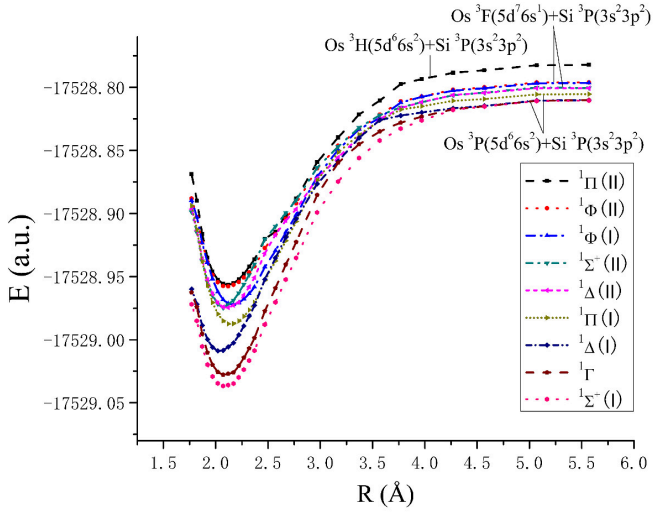

Figure S2: Potential Energy Curves of the Singlet States of OsSi.

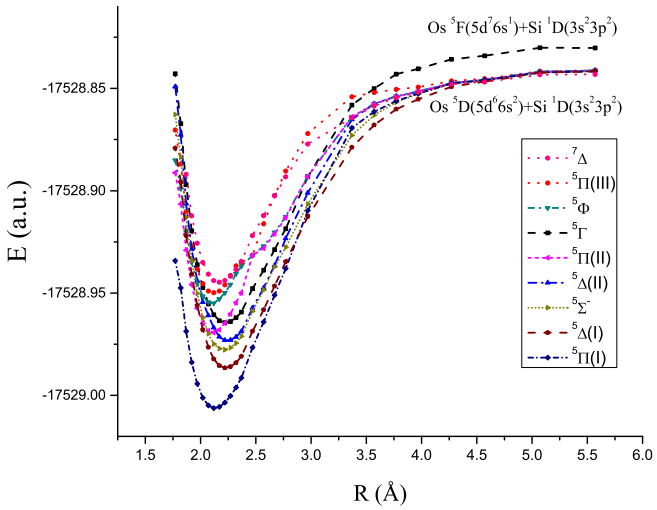

Figure S3: Potential Energy Curves of the Quintet and Septet States of OsSi.