

Empirical Tight-binding Parameterization of SmSe in the $sp^3d^5f^7s^*$ model

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Table 1 Diagonal and spin-orbit parameters for our parameterization of SmSe in the $sp^3d^5f^7s^*$ model. All values are in eV.

Parameter	SmSe
E_{sc}	40
E_{sa}	-8.2844
E_{pc}	20.3875
E_{pa}	4.3214
E_{dc}	10.1603
E_{da}	18.3778
E_{fc}	10.0915
E_{fa}	40
E_{s^*c}	10.8117
E_{s^*a}	31.8322
δ_{pc}	0.0046
δ_{pa}	0.3652
δ_{dc}	0.0769
δ_{da}	0.0174
δ_{fc}	2.0600
δ_{fa}	0

Table 2 First nearest neighbor two-center integrals for our parameterization of SmSe in the $sp^3d^5f^7s^*$ model. All values are in eV.

Parameter	SmSe
$ss\sigma$	-0.0004
$s^*s^*\sigma$	-0.1324
$s_c s^*_a$	0
$s^*_c s_a$	-0.0032
$s_a p_c \sigma$	0.1256
$s_c p_a \sigma$	0
$s^*_a p_c \sigma$	0.1726
$s^*_c p_a \sigma$	0.7035
$s_a d_c \sigma$	-1.9055
$s_c d_a \sigma$	0

$s^*_a d_c \sigma$	-0.0493
$s^*_c d_a \sigma$	-0.0111
$s_a f_c \sigma$	0
$s_c f_a \sigma$	0
$s^*_a f_c \sigma$	0.0002
$s^*_c f_a \sigma$	0
$pp\sigma$	0.1313
$pp\pi$	-0.1326
$p_a d_c \sigma$	-0.9865
$p_c d_a \sigma$	-0.9979
$p_a d_c \pi$	0.5711
$p_c d_a \pi$	0.8405
$p_a f_c \sigma$	-0.2168
$p_c f_a \sigma$	0
$p_a f_c \pi$	0.1982
$p_c f_a \pi$	0
$dd\sigma$	-0.5877
$dd\pi$	0.1156
$dd\delta$	-0.0942
$d_a f_c \sigma$	-0.0016
$d_c f_a \sigma$	0
$d_a f_c \pi$	0.00057
$d_c f_a \pi$	0
$d_a f_c \phi$	-0.00057
$d_c f_a \phi$	0
$ff\sigma$	0
$ff\pi$	0
$ff\delta$	0
$ff\phi$	0

Table 3 Second nearest neighbor two-center integrals for our parameterization of SmSe in the $sp^3d^5f^7s^*$ model. All values are in eV.

Parameter	SmSe
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$s_a s_a \sigma$	-0.0055
$s_c s_c \sigma$	0
$s^* a s^* a \sigma$	-0.0067
$s^* c s^* c \sigma$	-0.2457
$s_a s^* a$	-0.1173
$s_c s^* c$	0
$s_a p_a \sigma$	0.1833
$s_c p_c \sigma$	0.0007
$s^* a p_a \sigma$	0.1494
$s^* c p_c \sigma$	0.0717
$s_a d_a \sigma$	-0.0013
$s_c d_c \sigma$	0
$s^* a d_a \sigma$	-0.0079
$s^* c d_c \sigma$	-0.0033
$s_a f_a \sigma$	0
$s_c f_c \sigma$	0
$s^* a f_a \sigma$	0
$s^* c f_c \sigma$	0.0012
$p_a p_a \sigma$	0.2165
$p_c p_c \sigma$	1.0467
$p_a p_a \pi$	-0.0357
$p_c p_c \pi$	-0.1697
$p_a d_a \sigma$	-0.1523
$p_c d_c \sigma$	-0.2104
$p_a d_a \pi$	0.3064
$p_c d_c \pi$	0.0609
$p_a f_a \sigma$	0
$p_c f_c \sigma$	-0.0026
$p_a f_a \pi$	0
$p_c f_c \pi$	0.0008
$d_a d_a \sigma$	-0.1913
$d_c d_c \sigma$	-0.7889
$d_a d_a \pi$	0.3473
$d_c d_c \pi$	0.2889
$d_a d_a \delta$	-0.1749
$d_c d_c \delta$	-0.0805
$d_a f_a \sigma$	0
$d_c f_c \sigma$	-0.0310
$d_a f_a \pi$	0
$d_c f_c \pi$	0.0028
$d_a f_a \phi$	0
$d_c f_c \phi$	-0.0417
$f_a f_a \sigma$	0
$f_c f_c \sigma$	0
$f_a f_a \pi$	0
$f_c f_c \pi$	0

$f_a f_a \delta$	0
$f_c f_c \delta$	0
$f_a f_a \phi$	0
$f_c f_c \phi$	0

Table 4 Dimensionless scaling exponents, η , and diagonal parameter shift constants, C .

Parameter	SmSe
$\eta_{s^*s\sigma}$	2.7476
$\eta_{ss\sigma}$	1.1210
$\eta_{ss^*\sigma}$	2.7476
$\eta_{s^*s^*\sigma}$	0.3201
$\eta_{sp\sigma}$	1.9926
$\eta_{s^*p\sigma}$	7.4774
$\eta_{sd\sigma}$	2.8848
$\eta_{s^*d\sigma}$	0.4658
$\eta_{sf\sigma}$	2.6502
$\eta_{s^*f\sigma}$	1.8601
$\eta_{pp\sigma}$	0.5835
$\eta_{pp\pi}$	7.3834
$\eta_{pd\sigma}$	7.72240
$\eta_{pd\pi}$	0.2424
$\eta_{pf\sigma}$	3.7781
$\eta_{pf\pi}$	1.3919
$\eta_{dd\sigma}$	3.0106
$\eta_{dd\pi}$	3.7886
$\eta_{dd\delta}$	3.7201
$\eta_{df\sigma}$	1.6722
$\eta_{df\pi}$	0.0214
$\eta_{df\delta}$	0.3015
$\eta_{ff\sigma}$	2.0151
$\eta_{ff\pi}$	1.4708
$\eta_{ff\delta}$	0.8101
$\eta_{ff\phi}$	1.0060
E_{shift}	26.1099
$C_{sasc} C_{sasc}$	0.7263
C_{scsc}	1.0188
C_{sasa}	0.5019
$C_{s^*as^*c} C_{s^*cs^*a}$	0.7328
$C_{s^*cs^*c}$	0.3651
$C_{s^*as^*a}$	1.3870
C_{sas^*c}	1.0671
C_{scs^*a}	0.3292
C_{sas^*a}	0.6616
C_{scs^*c}	1.0432

C_{sapc}	0.9611
C_{sepa}	0.8207
C_{scpc}	1.1291
C_{sapa}	1.1030
C_{s*apc}	0.7722
C_{s*cpa}	6.1561
C_{s*cpc}	1.1660
C_{s*apa}	0.4389
C_{sadc}	1.1049
C_{scda}	0.9722
C_{scdc}	0.9030
C_{sada}	0.7891
C_{s*adc}	0.5091
C_{s*cda}	0.0488
C_{s*cdc}	0.7137
C_{s*ada}	0.7741
C_{safe}	1.1505
C_{sefa}	0.7301
C_{sefc}	1.2264
C_{safa}	1.2045
C_{s*afc}	0.5803
C_{s*cfa}	1.0349
C_{s*cfc}	0.8415
C_{s*afa}	0.4994
$C_{papc} C_{pcpa}$	4.5655
C_{pcpc}	4.8908
C_{papa}	2.4676
C_{padc}	0.0390
C_{pcda}	0.5881
C_{pcdc}	1.4889
C_{pada}	0.6510
C_{pafc}	7.0557
C_{pcfafa}	1.5457
C_{pcfafa}	0.8616
C_{pafa}	0.4083
$C_{dadc} C_{dcda}$	0.0111
C_{dcdc}	0.6516
C_{dada}	0.7797
C_{dafc}	1.7160
C_{dcfafa}	1.3235
C_{dcfc}	1.2333
C_{dafa}	0.9812
$C_{fafc} C_{fcfa}$	0.9665
C_{fcfc}	0.3764
C_{fafa}	1.5813
