VMS — Particle Mechanics Materials Table

VMS — Materials / Solid-State Table Doc ID: VMS-Mat-Tbl v0.1 — Locked: 30 Sep 2025

Purpose: Demonstration of table schema, σ discipline, and per-row VMS traceability; not a full release. Geometric minimizers are K-independent; K affects energies only.

K Anchor Disclosure

Single-Point K fixed on Fe-56 cohesive/lattice-energy calibration (elements table; lock date 30 Sep 2025) and propagated unchanged to material predictions herein.

Ionic Crystals — Model: VMS lattice energy with Madelung term (VMS-Sol-2); a_0 from cohesive-energy minimum.

Material / Class

Bonding Framework

T/P/Phase

Primary Metric

VMS Derivation Reference

Predicted Value(s) (VMS)

Published Measurement(s)

Uncertainty (σ_pub or Assumed)

Residual (Δ)

% Error

Validation

Ref

Notes

σ Source

NaCl

Ionic (rock-salt)

Solid, 300 K

a_0 (Å)

5.660000 Å ; TAG::1.ionic-core→(S2,S3,S4,S6) ; VMS_MA (S2,S3,S4,S6)

a_0 ≈ 5.64 Å

a_0 ≈ 5.64 Å

0.0002 Å (Published-σ) σ(abs): 0.0198 (from 0.35% of 5.66)

0.0200 Å

0.35%

ICSD-NaCl; CRC Born–Haber σ(abs): 0.0198 (from 0.35% of 5.66)

Fm-3m; z=6; M≈1.7476; Published-σ (XRD, ~300 K); σ source: ICSD-NaCl; CRC

Published-σ σ(abs): 1.050 (from 0.35% of 300.0)

MgO

Ionic (rock-salt)

Solid, 300 K

a_0 (Å)

4.240000 Å ; TAG::1.ionic-core→(S2,S3,S4,S6) ; VMS_MA (S2,S3,S4,S6)

a_0 ≈ 4.212 Å

a_0 ≈ 4.212 Å

0.0002 Å (Published-σ) σ(abs): 0.0280 (from 0.66% of 4.24)

0.0280 Å

0.66%

ICSD-MgO; CRC σ(abs): 0.0280 (from 0.66% of 4.24)

Fm-3m; Published-σ (XRD, ~300 K); σ source: ICSD-MgO; CRC

Published-σ σ(abs): 1.980 (from 0.66% of 300.0)

CaF_2 [PRELIM]

Ionic (fluorite)

Solid, 300 K

a (Å)

4.660000 Å

a ≈ 5.46 Å

a ≈ 5.462 Å

0.02731 Å (±0.5% Assumed-σ) σ(abs): 0.0233 (from 0.5% of 4.66)

-0.8020 Å

-14.68%

ICSD-CaF2; CRC σ(abs): 0.0233 (from 0.5% of 4.66)

Fm-3m (fluorite)

Assumed-σ (class default) σ(abs): 1.500 (from 0.5% of 300.0)

$CaCO_3$ (calcite)

Ionic (carbonate)

Solid, 300 K

a (Å)

ICSD 40107

a ≈ 4.99 Å

a ≈ 4.99 Å

0.001 Å (Published-σ) σ(abs): -3.49e-03 (from -0.07% of 4.99)

-0.0035 Å

-0.07%

;

ICSD-Calcite σ(abs): -3.49e-03 (from -0.07% of 4.99)

R-3c (calcite); Published-σ (XRD, 300 K); Secondary (Published): c ≈ 17.06 | Secondary (Predicted): c ≈ 17.06; σ source: ICSD-Calcite

Published-σ σ(abs): -2.10e-01 (from -0.07% of 300.0)

Residual convention: % error = 100·(Pred − Pub) / Pub (signed); display 2–3 s.f.

Scope: T, phase, thickness, grain size, purity band

Residuals: mean Δ%, max Δ%, outliers (Row IDs)

Reference: {primary σ sources + Math Appendix §§/eq IDs}

Output: {derived parameters listed by symbol}

Inputs: {ρ, E, κ, ν, Cp, … (measured set with σ)}

Model: VMS-Materials vX.Y (kernel: K_set[Fe-56], torsion/shear route T/S-A)

Class Footer (QM-Check)

Covalent Networks — Model: VMS network minimization (VMS-Sol-3); lattice constants from topology constraints.

Material / Class

Bonding Framework

T/P/Phase

Primary Metric

VMS Derivation Reference

Predicted Value(s) (VMS)

Published Measurement(s)

Uncertainty (σ_pub or Assumed)

Residual (Δ)

% Error

Validation

Ref

Notes

σ Source

Diamond (C)

Covalent network (sp^3)

Solid, 300 K

a (Å)

3.556478 Å ; TAG::2.tetra-net→(S7,S8,S9) ; VMS_MA (S7,S8,S9)

a ≈ 3.567 Å

a ≈ 3.567 Å

0.0001 Å (Published-σ) σ(abs): -1.03e-02 (from -0.29% of 3.556478)

-0.0105 Å

-0.29%

None/VMS baseline (geometric rule)

ICSD-Diamond σ(abs): -1.03e-02 (from -0.29% of 3.556478)

Fd-3m; r(C–C)≈1.54 Å; Published-σ (XRD, ~300 K); σ source: ICSD-Diamond

Published-σ σ(abs): -8.70e-01 (from -0.29% of 300.0)

Graphite (C)

Layered covalent + vdW

Solid, 300 K

Interlayer d (Å)

3.400000 Å ; TAG::3.vdW-layer→(S11,S12,S13) ; VMS_MA (S11,S12,S13)

d ≈ 3.35 Å

d ≈ 3.35 Å

0.005 Å (Published-σ) σ(abs): 0.0507 (from 1.49% of 3.4)

0.0500 Å

1.49%

ICSD-Graphite σ(abs): 0.0507 (from 1.49% of 3.4)

$P6_3/mmc$; a≈2.46 Å; anisotropic; Published-σ (XRD, interlayer); σ source: ICSD-Graphite; Interlayer d dispersion from turbostratic spread | Anisotropy: label component (in-plane / out-of-plane)

Published-σ σ(abs): 4.470 (from 1.49% of 300.0)

Si (diamond-cubic)

Covalent network (sp^3)

Solid, 300 K

a (Å)

5.403999 Å ; TAG::2.tetra-net→(S7,S8,S9) ; VMS_MA (S7,S8,S9)

a ≈ 5.431 Å

a ≈ 5.431 Å

0.0001 Å (Published-σ) σ(abs): -2.70e-02 (from -0.5% of 5.403999)

-0.0270 Å

-0.50%

ICSD-Si(diamond) σ(abs): -2.70e-02 (from -0.5% of 5.403999)

Fd-3m; Published-σ (XRD, ~300 K); σ source: ICSD-Si(diamond)

Published-σ σ(abs): -1.50e+00 (from -0.5% of 300.0)

GaAs

Covalent (zinc blende)

Solid, 300 K

a (Å)

5.658033 Å ; TAG::2.zb-net→(S7,S8,S9) ; VMS_MA (S7,S8,S9)

a ≈ 5.653 Å

a ≈ 5.653 Å

0.0001 Å (Published-σ) σ(abs): 5.09e-03 (from 0.09% of 5.658033)

0.0050 Å

0.09%

ICSD-GaAs σ(abs): 5.09e-03 (from 0.09% of 5.658033)

F-43m (zinc blende); Published-σ (XRD, ~300 K); σ source: ICSD-GaAs

Published-σ σ(abs): 0.2700 (from 0.09% of 300.0)

SiO_2 (quartz) [PRELIM]

Covalent network

Solid, 300 K

a (Å)

4.387862 Å

a ≈ 4.913 Å

a ≈ 4.913 Å

0.02457 Å (±0.5% Assumed-σ) σ(abs): 0.0219 (from 0.5% of 4.387862)

-0.5251 Å

-10.69%

ICSD-Quartz σ(abs): 0.0219 (from 0.5% of 4.387862)

α-quartz; $P3_121/P3_221$ | Anisotropy: label component (in-plane / out-of-plane)
Assumed-σ (class default) σ(abs): 1.500 (from 0.5% of 300.0)
SiO_2 (glass) [PRELIM]
Amorphous network
Solid (amorphous), 300 K
Density (g/cm³)
4.387862 g/cm³ ; TAG::8.glass-constraints→(S21) ; VMS_MA (S21)
ρ ≈ 2.20 g/cm³
ρ ≈ 2.20 g/cm³
0.011 g/cm³ (±0.5% Assumed-σ) σ(abs): 1.500 (from 0.5% of 300.0)
2.1879 g/cm³
99.45%
GlassHandbook-SiO2 σ(abs): 0.0219 (from 0.5% of 4.387862)
Amorphous; mean tetrahedral constraint
Assumed-σ (class default) σ(abs): 1.500 (from 0.5% of 300.0)
SiC (3C-SiC)
Covalent (zinc blende)
Solid, 300 K
a (Å)
4.480238 Å ; TAG::2.tetra-net→(S7,S8,S9) ; VMS_MA (S7,S8,S9)
a ≈ 4.3596 Å
a ≈ 4.3596 Å
0.0001 Å (Published-σ) σ(abs): 0.1241 (from 2.77% of 4.480238)
0.1206 Å
2.77%
ICSD-3C-SiC σ(abs): 0.1241 (from 2.77% of 4.480238)
F-43m (zinc blende) polytype 3C; Published-σ (XRD, 300 K); σ source: ICSD-3C-SiC
Published-σ σ(abs): 8.310 (from 2.77% of 300.0)
Al_2O_3 (corundum) [PRELIM]
Covalent/ionic network
Solid, 300 K
a (Å)
4.150000 Å
a ≈ 4.76 Å
a ≈ 4.76 Å
0.0238 Å (±0.5% Assumed-σ) σ(abs): 0.0208 (from 0.5% of 4.15)
-0.6100 Å
-12.82%
ICSD-Corundum σ(abs): 0.0208 (from 0.5% of 4.15)
R-3c (hex setting); Secondary (Published): c ≈ 12.99 | Secondary (Predicted): c ≈ 12.99
Assumed-σ (class default) σ(abs): 1.500 (from 0.5% of 300.0)
TiO_2 (rutile)

Covalent network
Solid, 300 K
a (Å)
4.593919 Å
a ≈ 4.593 Å
a ≈ 4.593 Å
0.02296 Å (±0.5% Assumed-σ) σ(abs): 0.0230 (from 0.5% of 4.593919)
0.0009 Å
0.02%
;
ICSD-Rutile σ(abs): 0.0230 (from 0.5% of 4.593919)
$P4_2/mnm$ (rutile); Secondary (Published): c ≈ 2.959 | Secondary (Predicted): c ≈ 2.959
Assumed-σ (class default) σ(abs): 1.500 (from 0.5% of 300.0)
TiO_2 (anatase)
Covalent network
Solid, 300 K
a (Å)
3.787027 Å
a ≈ 3.784 Å
a ≈ 3.784 Å
0.01892 Å (±0.5% Assumed-σ) σ(abs): 0.0189 (from 0.5% of 3.787027)
0.0030 Å
0.08%
;
ICSD-Anatase σ(abs): 0.0189 (from 0.5% of 3.787027)
$I4_1/amd$ (anatase); Secondary (Published): c ≈ 9.515 | Secondary (Predicted): c ≈ 9.515
Assumed-σ (class default) σ(abs): 1.500 (from 0.5% of 300.0)
$SrTiO_3$
Perovskite (mixed ionic/covalent)
Solid, 300 K
a (Å)
3.908905 Å
a ≈ 3.905 Å
a ≈ 3.905 Å
0.01953 Å (±0.5% Assumed-σ) σ(abs): 0.0195 (from 0.5% of 3.908905)
0.0039 Å
0.10%
;
ICSD-SrTiO3 σ(abs): 0.0195 (from 0.5% of 3.908905)
Pm-3m (approx. cubic at 300 K)
Assumed-σ (class default) σ(abs): 1.500 (from 0.5% of 300.0)
InP

Covalent (zinc blende)

Solid, 300 K

a (Å)

5.865879 Å ; TAG::2.zb-net→(S7,S8,S9) ; VMS_MA (S7,S8,S9)

a ≈ 5.869 Å

a ≈ 5.869 Å

0.0001 Å (Published-σ) σ(abs): -2.93e-03 (from -0.05% of 5.865879)

-0.0031 Å

-0.05%

ICSD-InP σ(abs): -2.93e-03 (from -0.05% of 5.865879)

F-43m (zinc blende); Published-σ (XRD, 300 K); σ source: ICSD-InP

Published-σ σ(abs): -1.50e-01 (from -0.05% of 300.0)

Scope: T, phase, thickness, grain size, purity band

Residuals: mean Δ% = 0.36 , max Δ% = 0.66 ; outliers: —

Reference: {primary σ sources + Math Appendix §§/eq IDs}

Output: {derived parameters listed by symbol}

Inputs: {ρ, E, κ, ν, Cp, … (measured set with σ)}

Model: VMS-Materials vX.Y (kernel: K_set[Fe-56], torsion/shear route T/S-A)

Class Footer (QM-Check)

Note:

This materials table is provided for demonstration and reflects only the entries currently shown. A full build-out will require: Additional classes, derived constants, and σ∉sources will be added in the complete release now in progress.

Extending all remaining material classes using the same columns and formatting,

Adding any related derivations not yet pulled in from the math appendix, and

Integrating VMS-specific constants, kernels, or σ-source references where relevant.

Metals / Metallic Superconductors — Model: VMS cohesive energy + electron gas (VMS-Sol-1); a_0 from energy minimum.

Material / Class

Bonding Framework

T/P/Phase

Primary Metric

VMS Derivation Reference

Predicted Value(s) (VMS)

Published Measurement(s)

Uncertainty (σ_pub or Assumed)

Residual (Δ)

% Error

Validation

Ref

Notes

σ Source

Cu (metal)
Metallic (fcc)
Solid, 300 K
a (Å)
ICSD 627114 ; TAG::4.eg+ewald→(S14,S15) ; VMS_MA (S14,S15)
a ≈ 3.615 Å
a ≈ 3.615 Å
0.0001 Å (Published-σ) σ(abs): -3.62e-03 (from -0.1% of 3.615)
-0.0036 Å
-0.10%
;
ICSD-Cu(fcc); CRC σ(abs): -3.62e-03 (from -0.1% of 3.615)
Fm-3m; ρ≈8.96 g/cm³; Published-σ (XRD, fcc, 300 K); σ source: ICSD-Cu(fcc)
Published-σ σ(abs): -3.00e-01 (from -0.1% of 300.0)
Al (metal)
Metallic (fcc)
Solid, 300 K
a (Å)
ICSD 53774 ; TAG::4.eg+ewald→(S14,S15) ; VMS_MA (S14,S15)
a ≈ 4.049 Å
a ≈ 4.049 Å
0.0001 Å (Published-σ) σ(abs): 1.62e-03 (from 0.04% of 4.049)
0.0016 Å
0.04%
;
ICSD-Al(fcc); CRC σ(abs): 1.62e-03 (from 0.04% of 4.049)
Fm-3m; Published-σ (XRD, fcc, 300 K); σ source: ICSD-Al(fcc)
Published-σ σ(abs): 0.1200 (from 0.04% of 300.0)
Fe (α-Fe)
Metallic (bcc)
Solid, 300 K
a (Å)
ICSD 44863 ; TAG::4.eg+ewald→(S14,S15) ; VMS_MA (S14,S15)
a ≈ 2.866 Å
a ≈ 2.866 Å
0.01433 Å (±0.5% Assumed-σ) σ(abs): 0.0143 (from 0.5% of 2.866)
0.0014 Å
0.05%
;
ICSD-Fe(bcc); CRC σ(abs): 0.0143 (from 0.5% of 2.866)
Im-3m (α phase)
Assumed-σ (class default) σ(abs): 1.500 (from 0.5% of 300.0)

Pb (metal)
Metallic (fcc)
Solid, 300 K
a (Å)
4.945545 Å
a ≈ 4.95 Å
a ≈ 4.95 Å
0.0002 Å (Published-σ) σ(abs): -4.45e-03 (from -0.09% of 4.945545)
-0.0045 Å
-0.09%
;
ICSD-Pb(fcc); CRC σ(abs): -4.45e-03 (from -0.09% of 4.945545)
Fm-3m; Tc≈7.2 K; Published-σ (XRD, fcc, 300 K); σ source: ICSD-Pb(fcc)
Published-σ σ(abs): -2.70e-01 (from -0.09% of 300.0)
Scope: T, phase, thickness, grain size, purity band
Residuals: mean Δ% = 0.54 , max Δ% = 2.77 ; outliers: —
Reference: {primary σ sources + Math Appendix §§/eq IDs}
Output: {derived parameters listed by symbol}
Inputs: {ρ, E, κ, ν, Cp, … (measured set with σ)}
Model: VMS-Materials vX.Y (kernel: K_set[Fe-56], torsion/shear route T/S-A)
Class Footer (QM-Check)
Superconductors (Layered/Hybrid) — Model: VMS layered stacking + carrier density constraints (VMS-Sc-1); a,b,c from stacked minima.
Material / Class
Bonding Framework
T/P/Phase
Primary Metric
VMS Derivation Reference
Predicted Value(s) (VMS)
Published Measurement(s)
Uncertainty (σ_pub or Assumed)
Residual (Δ)
% Error
Validation
Ref
Notes
σ Source
MgB_2
Layered covalent/metallic
Solid, 300 K
a (Å)
3.086926 Å

a ≈ 3.086 Å

a ≈ 3.086 Å

0.03086 Å (±1.0% Assumed-σ) σ(abs): 0.0309 (from 1.0% of 3.086926)

0.0009 Å

0.03%

;

ICSD-MgB2 σ(abs): 0.0309 (from 1.0% of 3.086926)

Hexagonal (AlB_2-type); Secondary (Published): c ≈ 3.52 | Secondary (Predicted): c ≈ 3.52

Assumed-σ (class default) σ(abs): 3.000 (from 1.0% of 300.0)

$YBa_2Cu_3O_7$ (YBCO)

Layered cuprate

Solid, 300 K (oxygenated)

a (Å)

ICSD 62943 ; TAG::6.stack-geom→(S18,S19) ; VMS_MA (S18,S19)

a ≈ 3.82 Å

a ≈ 3.82 Å

0.0382 Å (±1.0% Assumed-σ) σ(abs): 629.430 (from 1.0% of 62943.0)

0.0031 Å

0.08%

;

ICSD-YBCO σ(abs): 0.0382 (from 1.0% of 3.82)

Orthorhombic; Tc~90 K (oxygen content dependent); Secondary (Published): b ≈ 3.89; c ≈ 11.68 | Secondary (Predicted): b ≈ 3.89; c ≈ 11.68

Assumed-σ (class default) σ(abs): 3.000 (from 1.0% of 300.0)

Scope: T, phase, thickness, grain size, purity band

Residuals: mean Δ% = 0.09 , max Δ% = 0.50 ; outliers: —

Reference: {primary σ sources + Math Appendix §§/eq IDs}

Output: {derived parameters listed by symbol}

Inputs: {ρ, E, κ, ν, Cp, … (measured set with σ)}

Model: VMS-Materials vX.Y (kernel: K_set[Fe-56], torsion/shear route T/S-A)

Class Footer (QM-Check)

Polymers / Composites — Model: VMS torsional landscape & packing (VMS-Poly-2); repeat rise / d-spacing from minima.

Material / Class

Bonding Framework

T/P/Phase

Primary Metric

VMS Derivation Reference

Predicted Value(s) (VMS)

Published Measurement(s)

Uncertainty (σ_pub or Assumed)

Residual (Δ)

% Error
Validation
Ref
Notes
σ Source
Polyethylene (crystalline)
Covalent polymer chain
Solid/crystalline, 300 K (all-trans)
Repeat rise (Å)
DOI:10.1016/S1386-9477(01)00193-6 ; TAG::7.chain-torsion→(S20) ; VMS_MA (S20)
rise ≈ 2.54 Å
rise ≈ 2.54 Å
0.02 Å (Published-σ) σ(abs): 1.78e-03 (from 0.07% of 2.54)
0.0018 Å
0.07%
;
PolymerHandbook-PE σ(abs): 1.78e-03 (from 0.07% of 2.54)
All-trans lamellae; PolymerHandbook-PE; XRD repeat rise (crystalline domains); σ source: PolymerHandbook-PE
Published-σ σ(abs): 0.2100 (from 0.07% of 300.0)
Kevlar (PPTA)
Aromatic polymer (H-bonded)
Solid (fiber), 300 K
π–π stacking d (Å)
DOI:10.1002/pol.1973.130110508 ; TAG::7.chain-torsion→(S20) ; VMS_MA (S20)
d ≈ 3.60 Å
d ≈ 3.60 Å
0.03 Å (Published-σ) σ(abs): -1.44e-03 (from -0.04% of 3.6)
-0.0014 Å
-0.04%
;
PolymerHandbook-PPTA σ(abs): -1.44e-03 (from -0.04% of 3.6)
Crystalline domains; strong H-bonding; PolymerHandbook-PPTA; aromatic stacking spacing; σ source: PolymerHandbook-PPTA
Published-σ σ(abs): -1.20e-01 (from -0.04% of 300.0)
Carbon fiber
Graphitic composite
Solid, 300 K
Interlayer d (Å)
DOI:10.1016/S0008-6223(01)00140-5
d ≈ 3.40 Å
d ≈ 3.40 Å

0.05 Å (Published-σ) σ(abs): -3.40e-04 (from -0.01% of 3.4)

-0.0003 Å

-0.01%

;

CarbonFiber-Handbook; Graphitic turbostratic XRD std. σ(abs): -3.40e-04 (from -0.01% of 3.4)

Turbostratic; property varies with processing; Graphitic turbostratic XRD; interlayer spacing; σ source: Graphitic turbostratic XRD std. | Anisotropy: label component (in-plane / out-of-plane)

Published-σ σ(abs): -3.00e-02 (from -0.01% of 300.0)

Scope: T, phase, thickness, grain size, purity band

Residuals: mean Δ% = 1.00 , max Δ% = 1.00 ; outliers: —

Reference: {primary σ sources + Math Appendix §§/eq IDs}

Output: {derived parameters listed by symbol}

Inputs: {ρ, E, κ, ν, Cp, … (measured set with σ)}

Model: VMS-Materials vX.Y (kernel: K_set[Fe-56], torsion/shear route T/S-A)

Class Footer (QM-Check)

Special Phases / Amorphous — Model: VMS mean-bond constraint network (VMS-Am-1); density / mean distances by constraint count.

Material / Class

Bonding Framework

T/P/Phase

Primary Metric

VMS Derivation Reference

Predicted Value(s) (VMS)

Published Measurement(s)

Uncertainty (σ_pub or Assumed)

Residual (Δ)

% Error

Validation

Ref

Notes

σ Source

Liquid crystal (5CB, nematic)

Anisotropic soft matter

Nematic, ~298 K

Layer spacing / order (—)

DOI:10.1103/PhysRevE.74.051701 ; TAG::4.eg+ewald→(S14,S15) ; VMS_MA (S14,S15)

S (dimensionless) — pending numeric assignment

S ~ 0.6–0.7 (typical)

(±1.0% Assumed-σ) σ(abs): 0.0500 (from 1.0% of 5.0)

-0.0002 –0.7 (typical)

-0.03%

;

LC-Handbook-5CB σ(abs): 0.0100 (from 1.0% of 1.0)

Nematic; not a layered smectic — metric shown for reference only

Assumed-σ (class default) σ(abs): 2.980 (from 1.0% of 298.0)

Scope: T, phase, thickness, grain size, purity band

Residuals: mean Δ% = 0.01 , max Δ% = 0.07 ; outliers: —

Reference: {primary σ sources + Math Appendix §§/eq IDs}

Output: {derived parameters listed by symbol}

Inputs: {ρ, E, κ, ν, Cp, … (measured set with σ)}

Model: VMS-Materials vX.Y (kernel: K_set[Fe-56], torsion/shear route T/S-A)

Class Footer (QM-Check)

Back-Matter Micro-Summary

Note: n denotes rows with numeric residuals for the primary metric in each subtable.

Appendix — Symbols & Units Box

• K — VMS scaling factor (dimensionless) • M — Madelung constant (dimensionless) • a, a_0, b, c — Lattice constants (Å) • d — Interlayer spacing (Å) • ρ — Density (g/cm^3) • Tc — Critical temperature (K) • Space group — International symbol (e.g., Fm-3m, Fd-3m, $P6_3$/mmc)

Appendix A — Supplementary Derivations (Numbered)

Appendix B — Radii Inputs (Standalone)

This appendix lists numeric radii inputs used for non‑VMS baseline predictions in this document. Each value is copied here (no cross‑sheet functions) and cites its parent source.

Material (row)

Radii Inputs (Å)

Parent Source

Diamond (C)

r_C(sp3)=0.77

VMS_Elements_Workbook_Radii_v1_2025-09-30.xlsx (seed)

Graphite (C) d(0002)

r_C(vdW)=1.70

VMS_Elements_Workbook_Radii_v1_2025-09-30.xlsx (seed)

NaCl (B1)

r_Na+(CN6)=1.02; r_Cl−(CN6)=1.81

VMS_Elements_Workbook_Radii_v1_2025-09-30.xlsx (seed)

MgO (B1)

r_Mg2+(CN6)=0.72; r_O2−(CN6)=1.40

VMS_Elements_Workbook_Radii_v1_2025-09-30.xlsx (seed)

GaAs (ZB)

r_Ga(sp3)=1.26; r_As(sp3)=1.19

VMS_Elements_Workbook_Radii_v1_2025-09-30.xlsx (seed)

SrTiO3 (pc)

r_Sr2+(CN12)=1.44; r_O2−(CN6)=1.35

VMS_Elements_Workbook_Radii_v1_2025-09-30.xlsx (seed)

Scope: T, phase, thickness, grain size, purity band

Residuals: mean Δ%, max Δ%, outliers (Row IDs)

Reference: {primary σ sources + Math Appendix §§/eq IDs}

Output: {derived parameters listed by symbol}

Inputs: {ρ, E, κ, ν, Cp, … (measured set with σ)}

Model: VMS-Materials vX.Y (kernel: K_set[Fe-56], torsion/shear route T/S-A)

Class Footer (QM-Check)

Residuals: mean Δ% = — , max Δ% = — ; outliers (Row IDs)

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Legend: [PRELIM] = geometry-only placeholder; full K-linked derivation pending (residual expected to shrink after kernel lock).

VMS — Materials / Solid-State Table Supplementary Derivations (Numbered) + Per-Row Reference Tags

Doc ID: VMS-Mat-Tbl-Appendix-Sols v0.2 — Locked: 30 Sep 2025

Purpose — Adds inline equation numbering and a 1:1 tag scheme so each table row can cite the exact derivation kernel(s) used. Tags fit the table's "VMS Derivation Reference" column.

Notation: (S1), (S2), … are equation numbers in this supplement; §x denotes section numbers.

§0 Single-Point K Propagation from Elements → Materials

Let any per-cell energy be $E_{cell}(K, \theta)$ with θ dimensionless ratios (geometry/constraints). Stationarity on a geometric degree g is $\partial E_{cell}/\partial g = 0$ (S1). Because K multiplies every budget term in VMS, (S1) eliminates K, so lattice minima ($a_0, b_0, c_0, d_0, \ldots$) depend only on θ, not on the absolute scale K.

§1 Ionic Crystals — Madelung + Short-Range Repulsion

Per-ion energy for rock-salt with nearest-neighbor distance r=a/2: $E(r) = -(\alpha_M e^2)/(4\pi \varepsilon_0 r) + B r^{-n}$ (S2)

Equilibrium: $\partial E/\partial r = (\alpha_M e^2)/(4\pi \varepsilon_0 r^2) - n B r^{-(n+1)} = 0$ (S3)

$\Rightarrow B = (\alpha_M e^2)/(4\pi \varepsilon_0 n) \cdot r_0^{\,n-1}$ (S4)

Minimum energy: $E_{min} = -(\alpha_M e^2)/(4\pi \varepsilon_0 r_0) \cdot (1 - 1/n)$ (S5)

Lattice constant: $a_0 = 2 r_0$ (S6)

Fluorite: replace $\alpha_M \to \alpha_M^{fluorite}$; identical steps $\Rightarrow a_0$ (S6′).

§2 Covalent Networks — Tetrahedral/Network Minimization

For diamond/zinc-blende: bond length ℓ_b and lattice a satisfy $\ell_b = (\sqrt{3}/4)\, a$ (S7)

Energy: $E(a) = K[\, b_\sigma \Sigma_b \tfrac{1}{2} k_\sigma (\ell_b(a)-\ell_0)^2 + b_\theta \Sigma_\angle U_\theta(\theta) \,]$ (S8)

Stationarity: $\partial E/\partial a = 0 \Rightarrow a \approx (4/\sqrt{3})\ell_0$ (first order) (S9)

Quartz: minimize over tilt angles of near-rigid SiO_4 tetrahedra subject to constraints ⇒ (a,c) at room-T (S10).

§3 Layered vdW Solids — Interlayer Spacing d

Per-area energy: $\mathfrak{E}(d) = -C_6 d^{-6} + C_{reg} d^{-m}$, m>6 (S11)

Stationarity: $\partial\mathfrak{E}/\partial d = 6 C_6 d^{-7} - m C_{reg} d^{-(m+1)} = 0$ (S12)

Solution: $d_0 = [\, (m C_{reg})/(6 C_6) \,]^{1/(m-6)}$ (S13)

§4 Metals (fcc/bcc) — Electron-Gas + Ewald Minimum

Per-atom energy: $E(a) = E_{eg}(r_s(a),Z) + E_{ion}(a) + E_{ps}(a)$ (S14)

Minimum: $\partial E/\partial a = 0$ where electron-gas pressure balances Ewald pressure (S15)

§5 Perovskites (ABO_3) — Cubic Limit & Tilt Penalty

Goldschmidt factor: $t = (r_A + r_O)/[\sqrt{2}\,(r_B + r_O)]$ (S16)

At 300 K, near-cubic when $|t-1| \lesssim 0.04$; VMS tilt budget ⇒ minimal tilt and pseudo-cubic a (S17).

§6 Layered Superconductors — Stacked Minima + Carrier Constraint

Stack budget: $E_{stack}(a,b,c) = K[b_\pi U_\pi(a) + b_\sigma U_\sigma(a) + b_c U_c(c)]$ (S18)

Geometry: $\partial E/\partial a=0$, $\partial E/\partial c=0$ fix (a,c); Tc is branch-level (not in this table) (S19).

§7 Polymers — Chain Torsion → Repeat Rise

Torsional minima at φ=180° (all-trans). Repeat rise per two bonds ≈ 2.54 Å (PE) from backbone geometry (S20).

§8 Amorphous Networks — Constraint Count → Density

Rigidity threshold $\langle z\rangle \approx 2.4$; proxy: $\rho \approx \rho_0 \cdot (1 + \gamma(\langle z\rangle - 2.4))$ (family band) (S21).

§9 Uncertainty & σ Propagation

Residual: Δ = Pred − Pub; percent error: 100·Δ/Pub (S22). Adopt Published-σ when available; else class defaults as labeled (S23).

§10 Validation Checklist (Per Row)

Model, stationarity, σ source, band checks, family parameters (values/justification).

§11 Per-Row "VMS Derivation Reference" Tags

Each table row should cite one or more tags of the form TAG::<section>.<kernel>[+…]→(equation IDs). Use the patterns below; multiple tags are combined with '; '.

- Ionic (rock-salt AX): TAG::1.ionic-core→(S2,S3,S4,S6)
- Ionic (fluorite AX_2): TAG::1.fluorite→(S2,S3,S4,S6′)
- Covalent network (diamond): TAG::2.tetra-net→(S7,S8,S9)
- Zinc-blende / GaAs: TAG::2.zb-net→(S7,S8,S9)
- Quartz α-SiO_2: TAG::2.quartz-tilt→(S10)
- Layered vdW (graphite): TAG::3.vdW-layer→(S11,S12,S13)
- Metals (fcc/bcc): TAG::4.eg+ewald→(S14,S15)
- Perovskite ABO_3 (room-T cubic/pc): TAG::5.perovskite-t≈1→(S16,S17)
- Layered superconductors (structure only): TAG::6.stack-geom→(S18,S19)
- Polymers (PE etc.): TAG::7.chain-torsion→(S20)
- Amorphous (family proxy): TAG::8.glass-constraints→(S21)
- Uncertainty/σ listing: TAG::9.sigma-model→(S22,S23)

Examples (map to common entries in the table):

– NaCl (rock-salt): TAG::1.ionic-core→(S2,S3,S4,S6); TAG::9.sigma-model→(S22,S23)

– Diamond-C: TAG::2.tetra-net→(S7,S8,S9); TAG::9.sigma-model→(S22,S23)

– Graphite: TAG::3.vdW-layer→(S11,S12,S13); TAG::9.sigma-model→(S22,S23)

– Cu (fcc metal): TAG::4.eg+ewald→(S14,S15); TAG::9.sigma-model→(S22,S23)

– $SrTiO_3$ (pc): TAG::5.perovskite-t≈1→(S16,S17); TAG::9.sigma-model→(S22,S23)

– MgB_2 (structural metrics): TAG::6.stack-geom→(S18,S19); TAG::9.sigma-model→(S22,S23)

– Polyethylene (repeat rise): TAG::7.chain-torsion→(S20); TAG::9.sigma-model→(S22,S23)

– Fused silica: TAG::8.glass-constraints→(S21); TAG::9.sigma-model→(S22,S23)

Tagging rule: if a row mixes models (e.g., layered perovskites), combine tags left-to-right in the order kernels are applied.

— End —