# Solving the phase boundary between two solid phases

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## Outline

F(V), G(P) and pressure of intersection. Thermal evolution

Shapes of G, F,  $\mathcal{E}$ 

Shape of H(P; T)

Phase Boundary

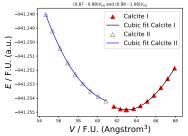
# Outline I

F(V), G(P) and pressure of intersection. Thermal evolution

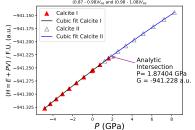
Shapes of G, F,  $\mathcal{E}$ 

Shape of H(P; T)

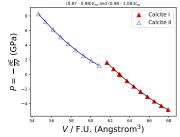
Phase Boundary



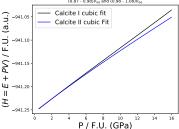
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8 (0.87 - 0.98)V<sub>ro</sub> and (0.98 - 1.08)V<sub>ro</sub>

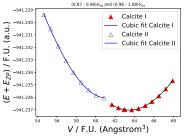


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

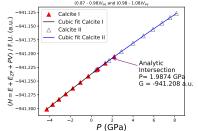


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8 (0.87 - 0.98)V<sub>eq</sub> and (0.98 - 1.08)V<sub>eq</sub>

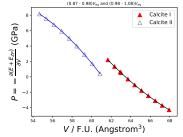




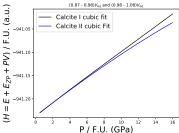
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8 (0.87 - 0.98)V<sub>ro</sub> and (0.98 - 1.08)V<sub>ro</sub>



PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

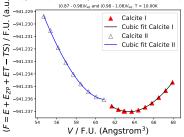


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8 (0.87 - 0.98)V<sub>eq</sub> and (0.98 - 1.08)V<sub>eq</sub>

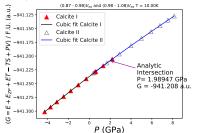


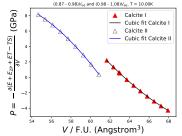
#### T = 10.00K

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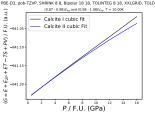


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



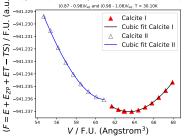


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

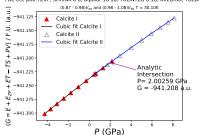


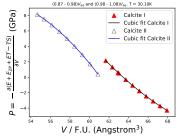
#### T = 30.10K

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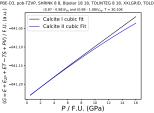


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



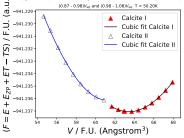


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

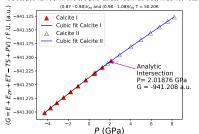


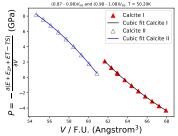
#### T = 50.20K

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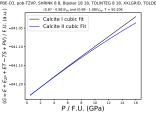


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



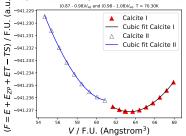


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

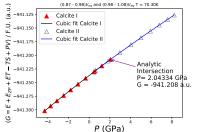


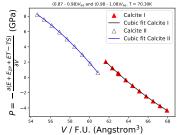
### T = 70.30K

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8  $(0.87 - 0.98)V_{eq}$  and  $(0.98 - 1.08)V_{eq}$ . T = 70.30K

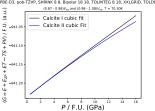


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



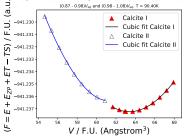


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

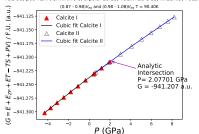


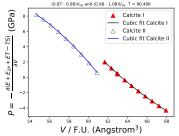
#### T = 90.40K

₱8E-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8  $(0.87 - 0.98)V_{eq}$  and  $(0.98 - 1.08)V_{eq}$ . T = 90.40K

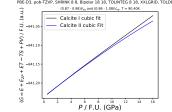


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



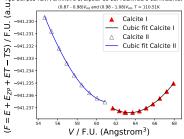


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

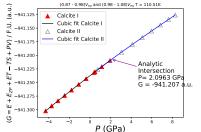


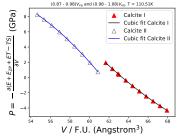
#### T = 110.51K

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

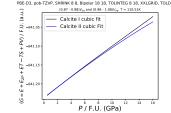


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



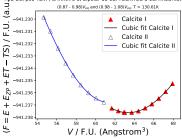


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

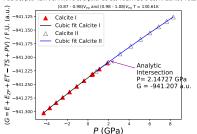


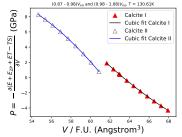
### T = 130.61K

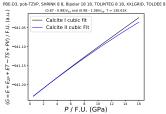
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

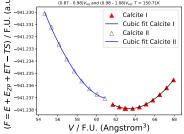




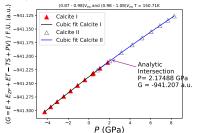


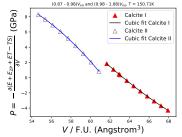
### T = 150.71K

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8 ⊐  $(0.87 - 0.98)V_{eq}$  and  $(0.98 - 1.08)V_{eq}$ . T = 150.71K

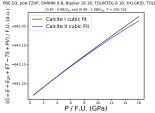


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



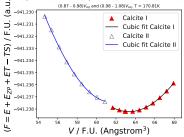


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

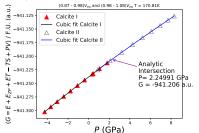


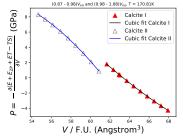
### T = 170.81K

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8  $(0.87 - 0.98)V_{eq}$  and  $(0.98 - 1.08)V_{eq}$ . T = 170.81K

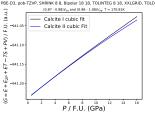


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



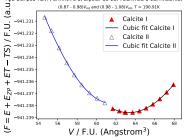


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

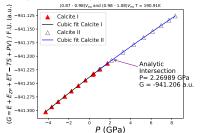


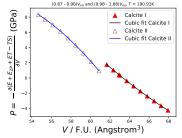
#### T = 190.91K

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

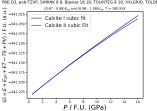


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

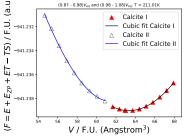




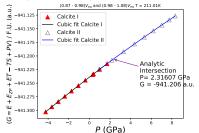
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



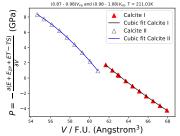
#### T = 211.01K



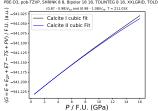
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

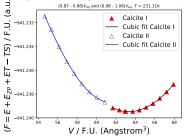


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

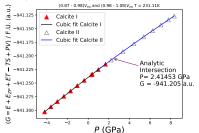


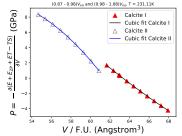
#### T = 231.11K

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

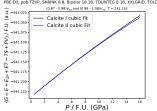


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



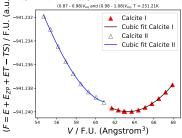


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

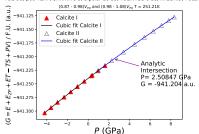


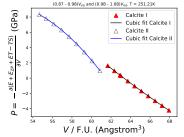
#### T = 251.21K

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

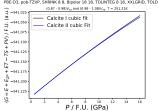


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



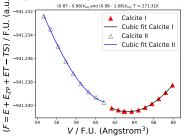


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

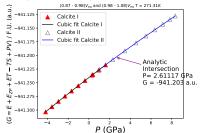


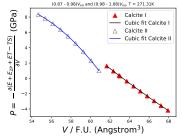
#### T = 271.31K

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

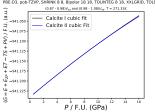


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



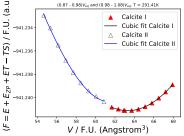


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

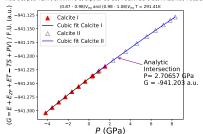


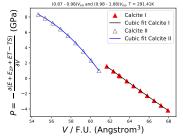
#### T = 291.41K

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

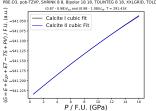


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

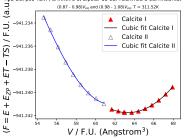




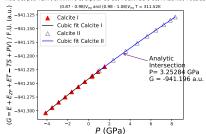
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



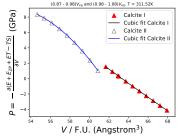
#### T = 311.52K



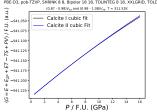
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



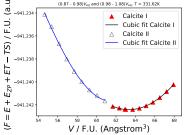
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



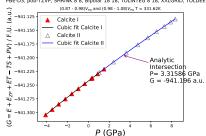
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



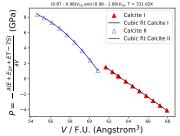
#### T = 331.62K



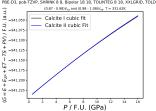
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

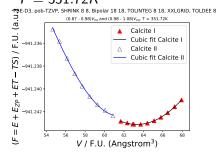


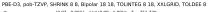
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

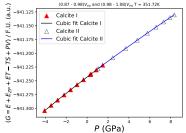


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

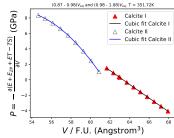












# Outline I

F(V), G(P) and pressure of intersection. Thermal evolution

Shapes of G, F,  $\mathcal{E}$ 

Shape of H(P; T)

Phase Boundary

#### T = 291.41 KPBE-D3, poin-TZVP, SHRIMK 8 6, Bipolar 18 18, TOUNTEG 8 18, XXLGRID, TOLDEE 8 PBE-D3, poin-TZVP, SHRINK 8 8, Bipolar 18 18, TOUNTEG 8 16, XXLGRID, TOLDEE 8 $(0.87 \cdot 0.98)V_{\rm eq}$ and $(0.58 \cdot 1.08)V_{\rm eq}$ T = 291.416 ▲ Calcite I - Cubic fit Calcite I △ Calcite II Cubic fit Calcite II ± 0.0000 E 0.0084 ▲ Calcite I £ .... - Cubic fit Calcite I △ Calcite II 0.0000 Cubic fit Calcite V / F.U. (Angstrom<sup>3</sup>) V / F.U. (Angstrom<sup>3</sup>) T = 311.52K: PRE-DS, poly-TZVP, SHAWK B & Blocker 18 18, TOLINTEG B 18, XXLGRID, TOLDEE B PRE-DS, poly-TZVF, SHRINK B & Blocker 18 18, TOLINTEG B 18, XXLGRID, TOLDEE B 10.07 - 8.90(4); and 10.90 - 1.60(4); T = 311.52K (ILEZ - 0.98 M<sub>cs</sub> and (ILEG - 1.08 M<sub>cs</sub>, T = 311.524) ▲ Calcite I ▲ Calcite I Cubic fit Calcite I Cubic fit Calcite I △ Calcite II △ Calcite II Cubic fit Calcite II Cubic fit Calcite II <u>s</u> .... € 0.0852 E .... V / F.U. (Angstrom<sup>3</sup>) V / F.U. (Angstrom<sup>3</sup>) T = 331.62K: SHRINK 6 6. Blooker 18 16. TOLINTOG 6 16. XXLGRID. TOLDES 6 10.87 - 8.8894., and 10.98 - 1.8894... T = 323.624 ▲ Calcite I ▲ Calcite I Cubic fit Calcite I Cubic fit Calcite I △ Calcite II △ Calcite II Cubic fit Calcite I Cubic fit Calcite II <u>6</u> 0.005 ₫ 0.0050 ⊒ 0.0050 0.0056 0.005 V / F.U. (Angstrom<sup>3</sup>) V / F.U. (Angstrom<sup>3</sup>) T = 351.72K: ▲ Calcite I Calcite I Cubic fit Calcite I Cubic fit Calcite I △ Calcite II △ Calcite II Cubic fit Calcite II Cubic fit Calcite II 9000 ⊒ 0.084 ⊃ 0.0064 . .... 0.0063

0.0061

V / F.U. (Angstrom<sup>3</sup>)

V / F.U. (Angstrom<sup>3</sup>)

ė 3

# Outline I

F(V), G(P) and pressure of intersection. Thermal evolution

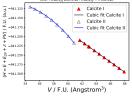
Shapes of G, F,  $\mathcal{E}$ 

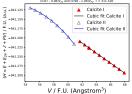
Shape of H(P; T)

Phase Boundary

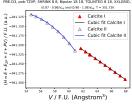
#### When $H(P; T) = E + E_{ZP} + \mathcal{E}(T) + PV$ :

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8 PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8 (0.87 - 0.98)V<sub>ec</sub> and (0.98 - 1.08)V<sub>ec</sub>, T = 291.41K (0.87 - 0.98)V<sub>cc</sub> and (0.98 - 1.08)V<sub>cc</sub>, T = 311.52K





PBE-D3, pob-TZVP, SHRINK 8 8, Bipplar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



# Outline I

F(V), G(P) and pressure of intersection. Thermal evolution

Shapes of G, F,  $\mathcal{E}$ 

Shape of H(P; T)

Phase Boundary

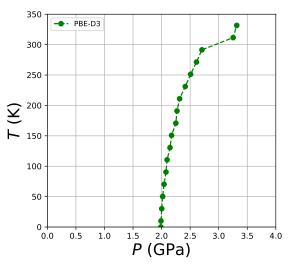


Figure 1: Pressure-temperature phase boundary