

HPC as a cost-effective complement to lab-science in materials research

JAVIER A. MONTOYA MARTÍNEZ

UNIVERSIDAD DE CARTAGENA - GRUPO DE MODELADO COMPUTACIONAL

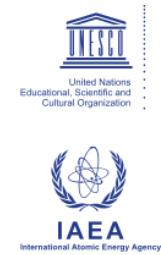


Universidad
de Cartagena

Fundada en 1827



The Abdus Salam
**International Centre
for Theoretical Physics**



University of Cartagena



Piedra de Bolívar



Zaragocilla
Pablo



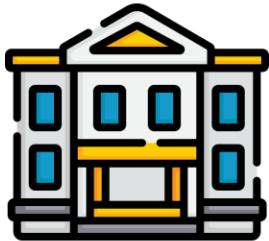
La Merced



San

Agustín

University of Cartagena



5 Campuses



6 Tutorial Centers



10 Schools



5 Institutes



104 Research Groups

University of Cartagena



36 005 Students



39 Undergrad



32 163 Undergrad
Students



34 Specializations



1 200 Professors



31 Masters



706 Employees



9 Ph. D. Programs

Universidad de Cartagena

Grupo de Modelado Computacional **COL0101016**



GruMoC in Numbers

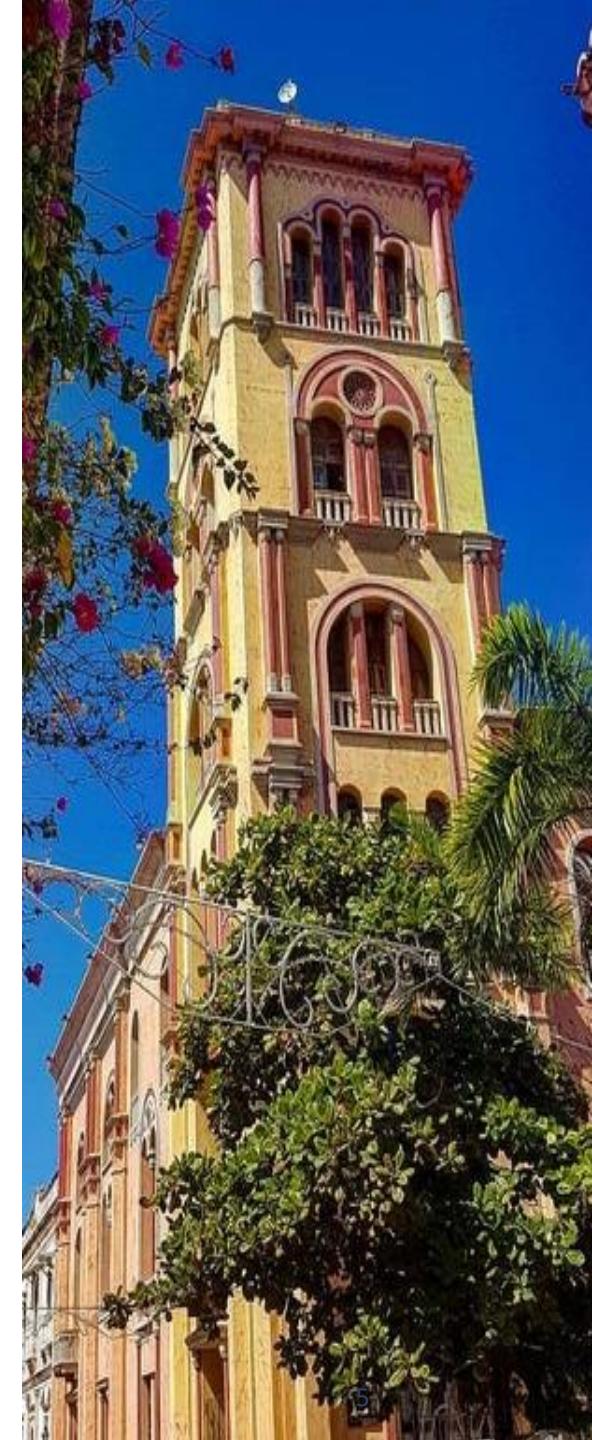
- Category A1 (Convocatoria 894 de 2021)
- Creation: Feb-2008

Members

- Professors: 4
- Post-docs: 1
- Ph. D. Students: 2
- M. Sc. Students: 2
- Undergrad Students: 2

Academic Production

- Scientific Articles: 90+
- Scientific Events: 140+
- Research Projects: 40+



University of Cartagena - HPC Systems



HPC Resource for Optics, Statistical Mechanics, Materials, and Energy - ROSMME

Commissioned in 2018, it is composed of the following servers:

- 1 x DELL PowerEdge-R330 1xIntel(R) Xeon(R) CPU E3-1225 v5 @ 3.30GHz - 8 Cores RAM 15 GB
- 5 x DELL PowerEdge R730 2xIntel(R) Xeon(R) CPU E5-2640 v4 @ 2.40GHz - 40 Cores RAM 125 GB
- 1 x DELL PowerEdge R640 2xIntel(R) Xeon(R) CPU Gold 6152 @ 2.10GHz -- 88 Cores RAM 314 GB
- Total Cores: (CPU Cores 296)
- Network: 1 x 40Gb Infiniband SWITCH, 1 x 10 Gb SWITCH, 1 x 1Gb fast-ETH SWITCH

University of Cartagena - Data Center



- Infrastructure known as TIER II due to its double redundancy.
- The Data Center was sold and installed by Hewlett Packard Enterprise with very high specifications.
- It was commissioned in 2019 and is currently in optimal operational conditions, serving as a vital starting point for hosting the new critical high-performance computing solutions required by the University of Cartagena.

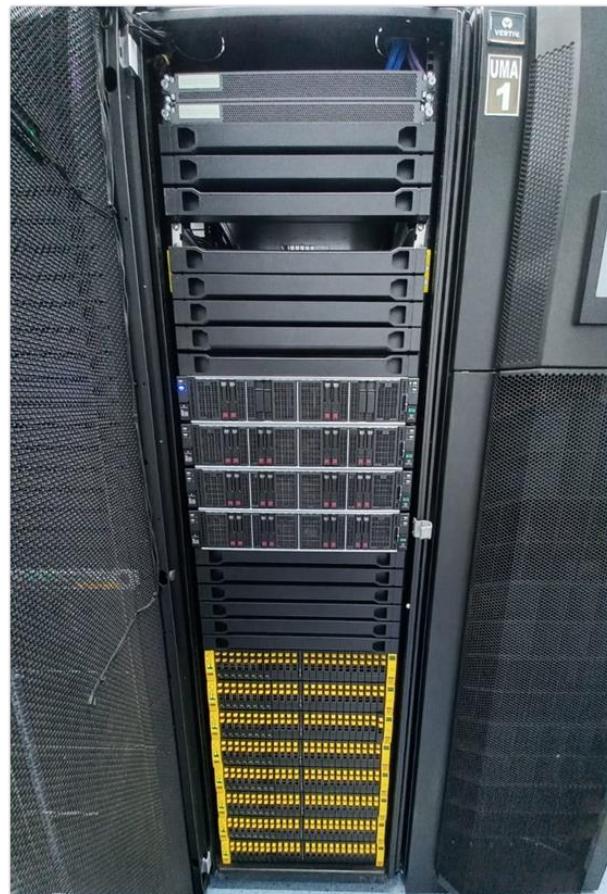
University of Cartagena - Virtualization



HP Synergy 480 G10 equipment with the following configuration:

- Two processors 6148 Xeon-G Kit (20C, 2.4GHz, 150W)
- 512 GB RAM
- HDD 300GB 12G SAS 10K 2.5in
- 8G LAN/SAN network interface
- Storage 3PAR-8400-4N

University of Cartagena - HPC Systems



Plataforma Avanzada de Cómputo para Ciencias Aplicadas - PACCA

Commissioned in 2023, it is composed of the following servers:

- 1 x HPE ProLiant XL290n Gen10 Plus 2xIntel Xeon-Gold 5317 @ 3.0GHz - 48 Cores RAM 256 GB
- 1 x HPE ProLiant XL290n Gen10 Plus 2xIntel Xeon-Gold 5315Y @ 3.2GHz - 32 Cores RAM 256 GB + GPU A100
- 12 x HPE ProLiant XL220n Gen10 Plus 2xIntel Xeon-Gold 5320 @ 2.2GHz - 104 Cores RAM 256 GB
- Total Cores: (CPU Cores 1,328)
- Network: 1 x 100Gb Infiniband SWITCH, 1 x ARUBA 1Gb fast-ETH

ICTP - HPC System Argo



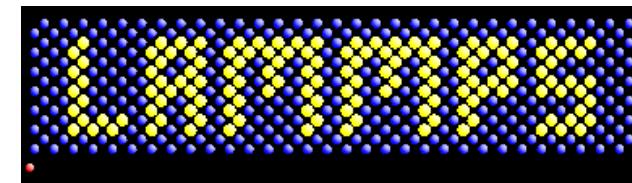
Argo is the ICTP general purpose HPC cluster, comprising:

- 153 hosts/nodes, with total count of 2588 CPUs
- Nearly 10 TB of memory
- 40Gbps+ InfiniBand interconnects
- 1Gbps network
- Several hundreds of TB of dedicated NFS storage

Parallel software tools



ENVIRON



The Latin America High Performance Computing Conference comes to Colombia

CARLA is an international conference aimed at providing a forum to foster the growth and strength of the High Performance Computing (HPC) community in Latin America through the exchange and dissemination of new ideas, techniques, and research in HPC and its applications areas. Started in 2014.

CARLA has become the flagship conference for HPC in the region. We invite the international community to share its advances on both HPC and HPC&AI (convergence between HPC and Artificial Intelligence) as those two key areas are becoming the predominant engine for innovation and development.

In 2023, the Latin America High Performance Computing Conference (CARLA 2023) will be from Cartagena de Indias, Colombia from September 18 -22, 2023. We expect contributions from faculty members, researchers, specialists and graduate students around the world.



Universidad
de Cartagena
Fundada en 1827



DIAMOND SPONSOR

DELL Technologies

AMD

www.carla2023.org



OUTLINE

Motivation

Introduction

Melting Curves and Limitations for Precise Calculations

Quasi-Harmonic Approximation (QHA)

Lindemann's Criteria

Identifying Melting Conditions on Carbon Phases

Applicability Beyond Carbon

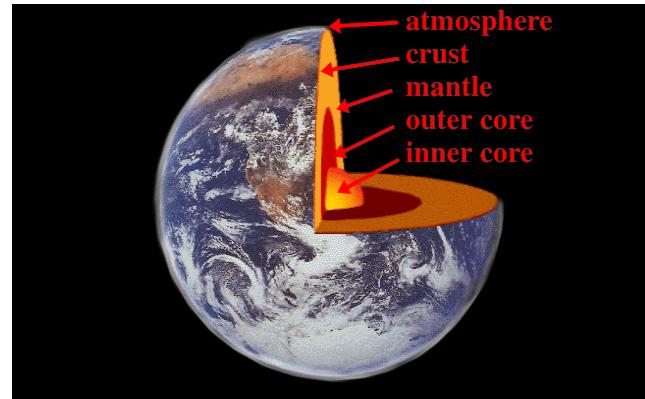
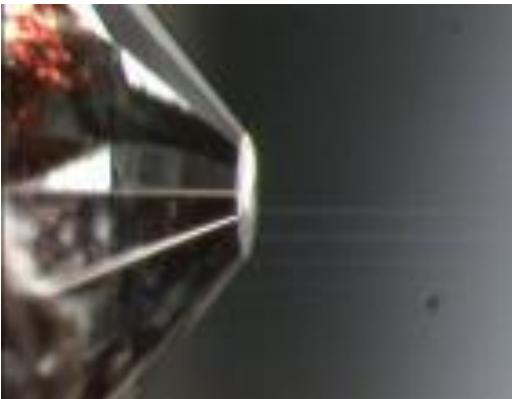
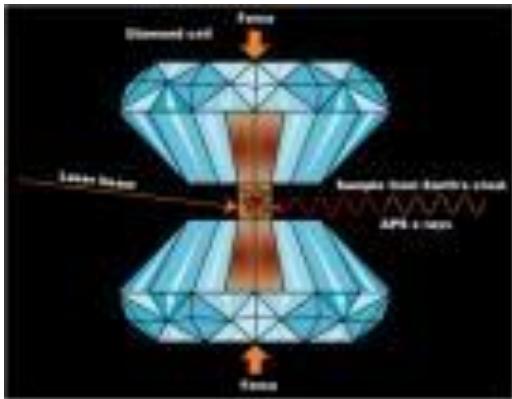
How it's done

Summary

Motivation

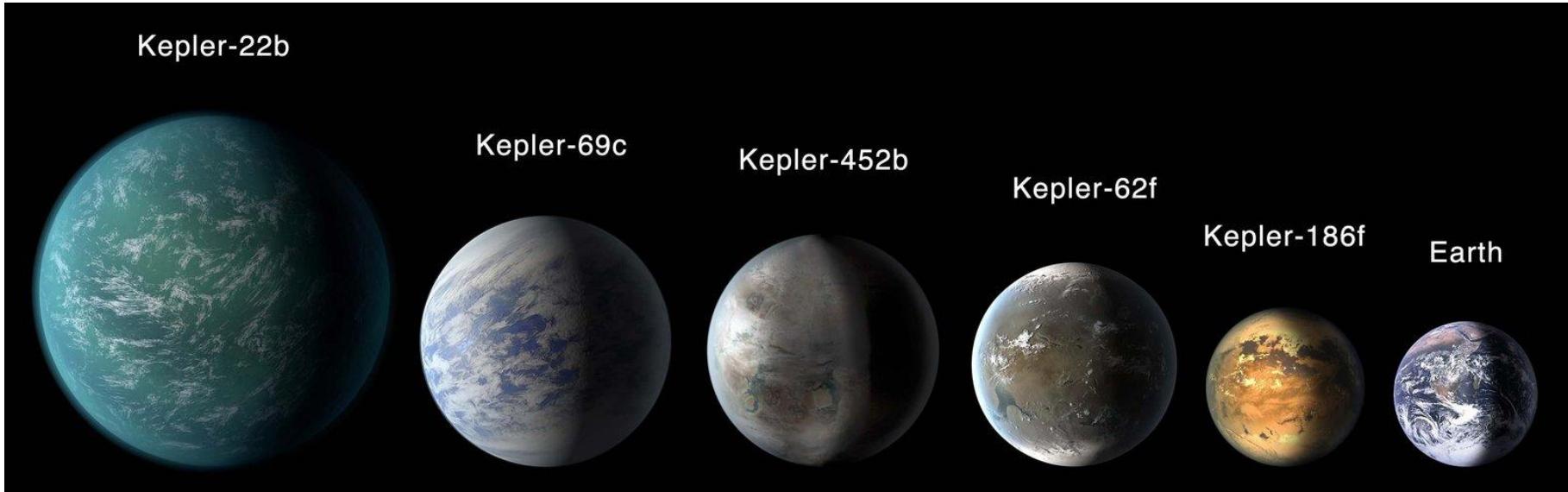
WHY HIGH PRESSURE?

Why we study materials at high-pressure?



- **Fundamental:** Effects of pressure on structure and bonding is still unknown in many cases.
- **Geological:** The study of minerals at high pressure is a wide open area: Chemistry of the planets, Earth's lower mantle.
- **Materials:** Pressure as a synthetic tool to new materials: Synthetic diamonds, high energy-density materials, new superconductors, etc.

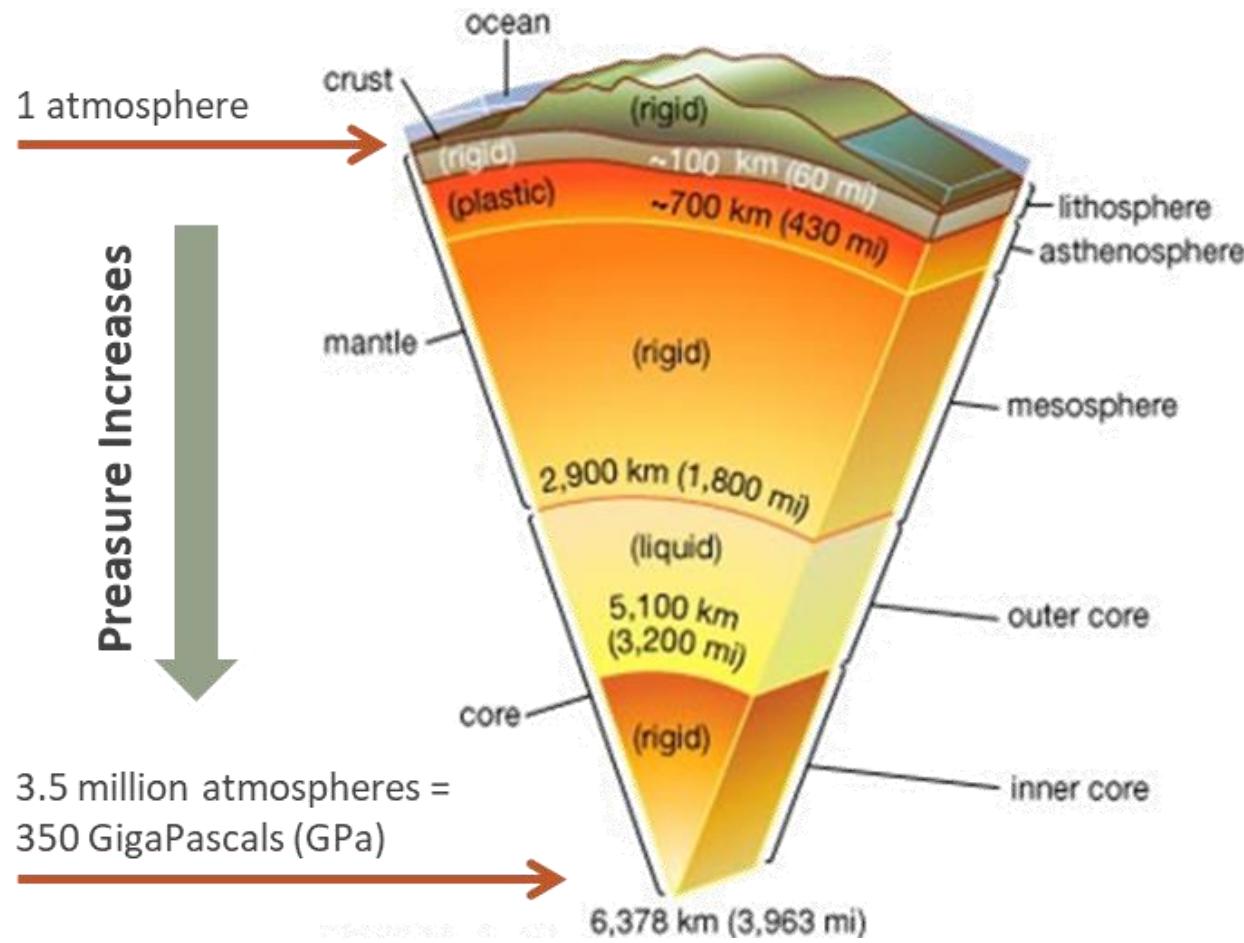
Why we study materials at high-pressure?



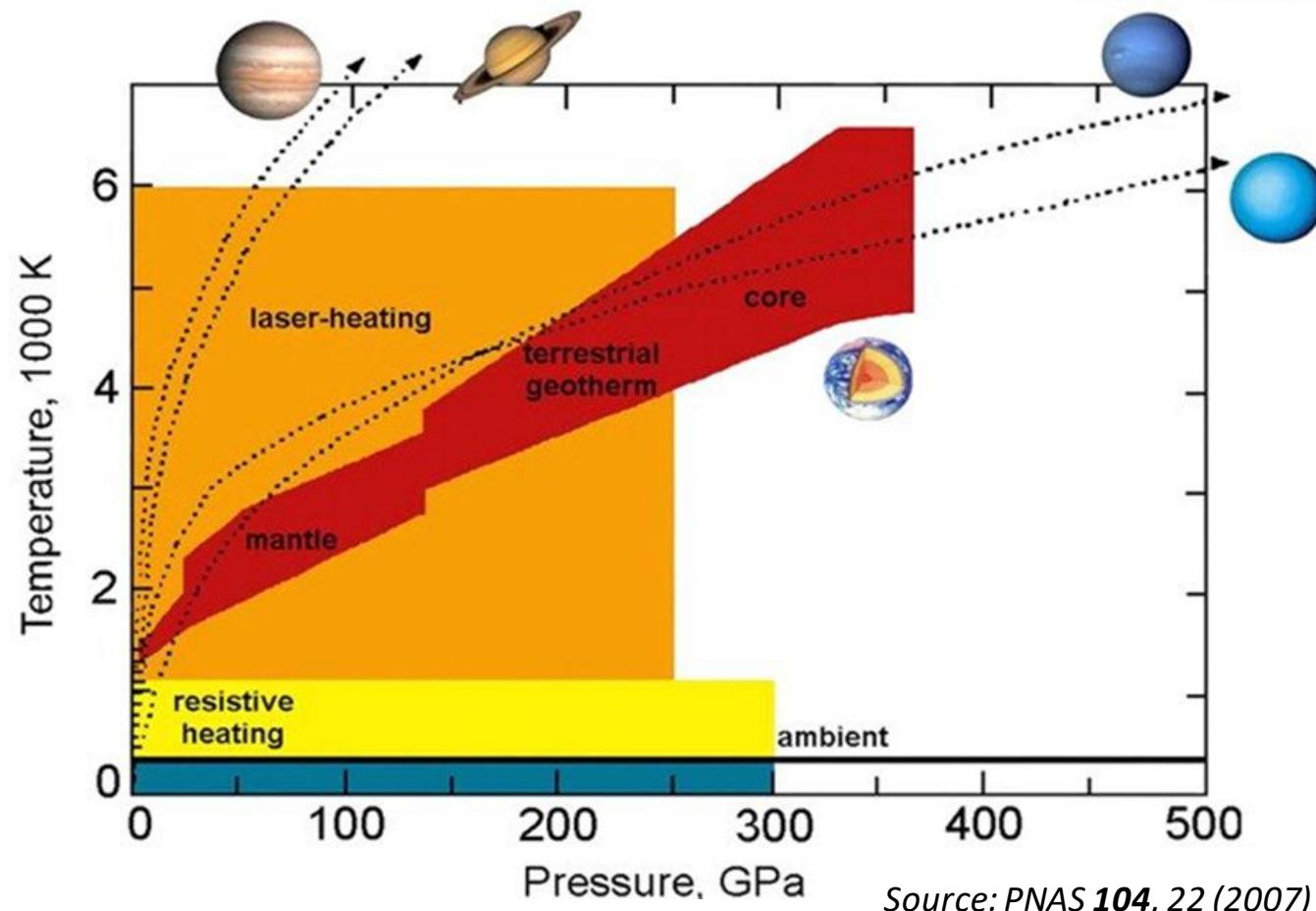
Source: Caltech

- **Geological:** The study of minerals at high pressure is a wide open area: Chemistry of the planets, Earth's lower mantle.

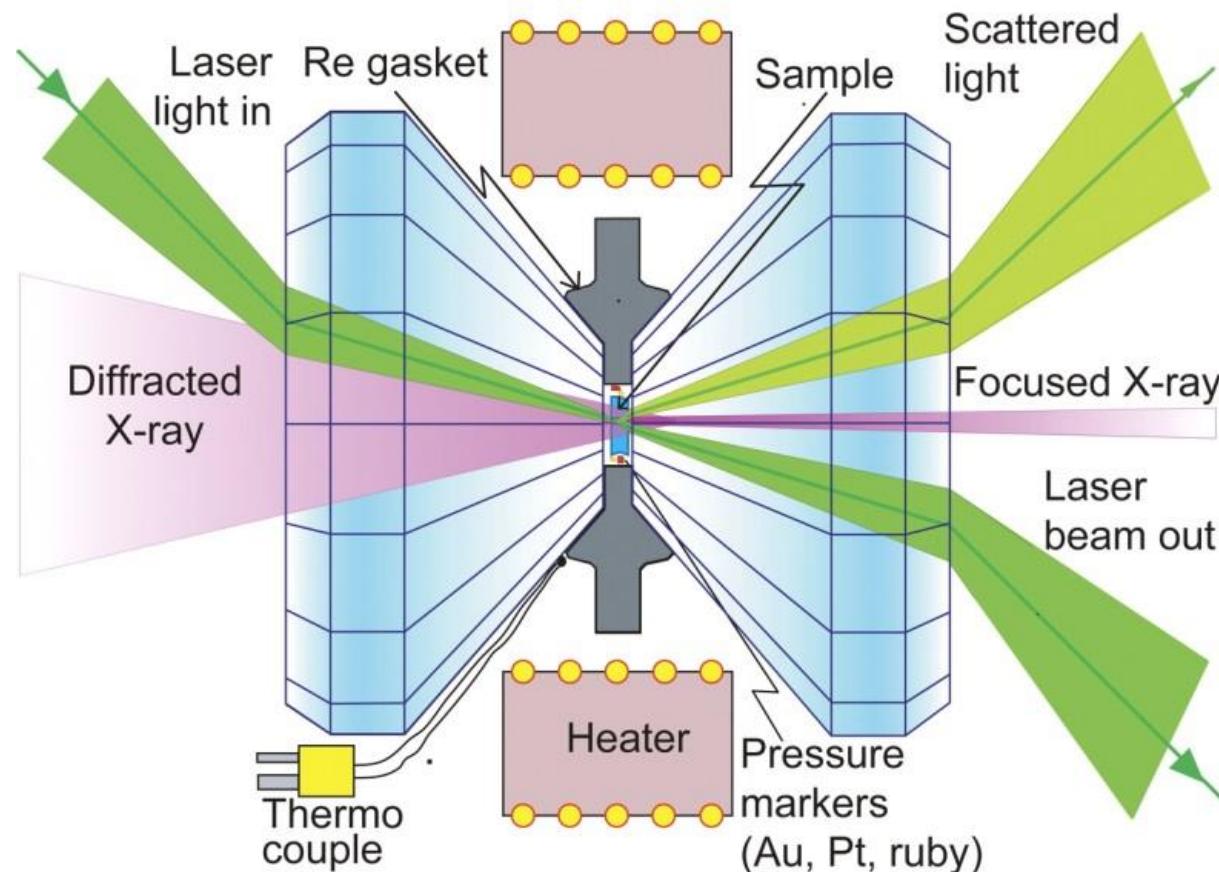
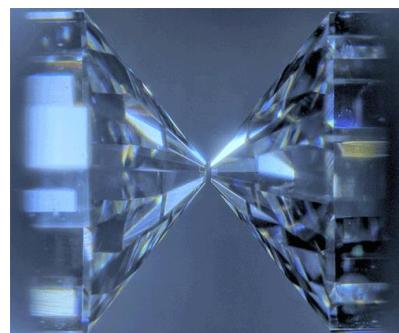
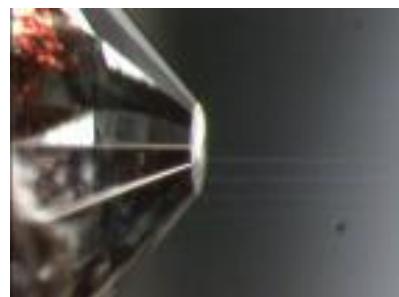
High-pressure on Earth



High-pressure on our Solar System



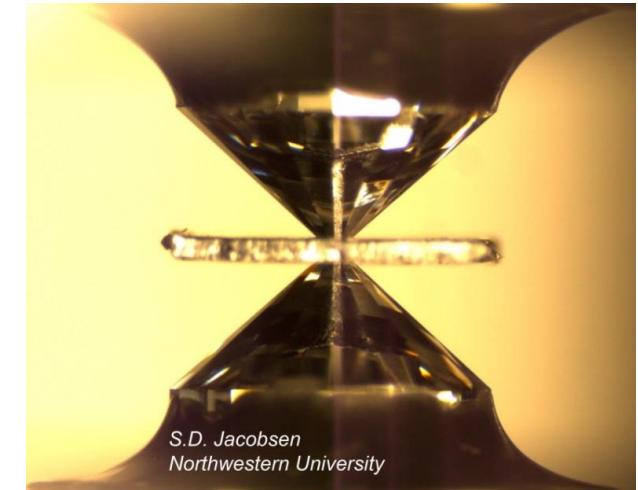
High-pressure in the laboratory



Source: SERC

The Diamond Anvil Cell (DAC) is an arrangement of counterpoised diamonds in the middle of which the samples are deposited.

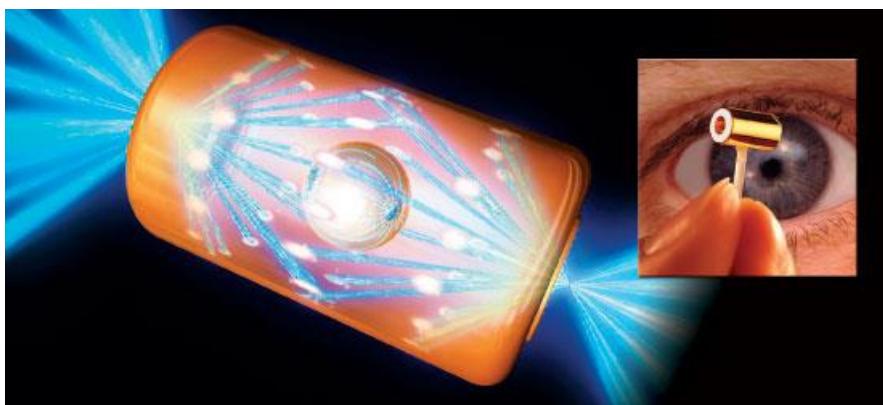
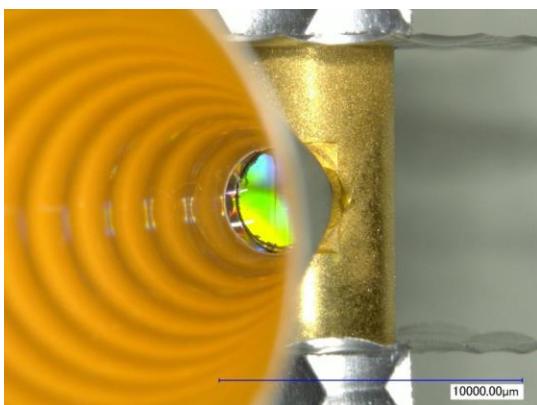
High-pressure in the laboratory



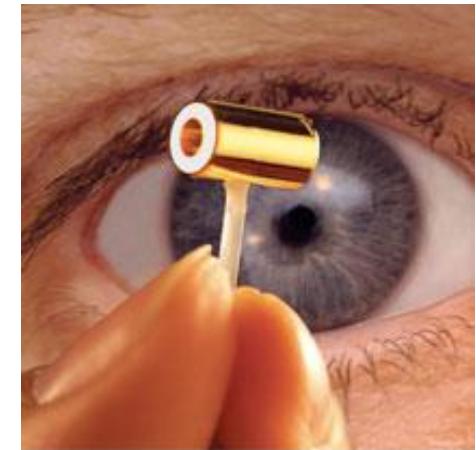
Highest pressures in a lab facility



On the Path to Ignition



Highest pressures in a lab facility



A National Ignition Facility (NIF) hohlraum. (NIF/LLNL)

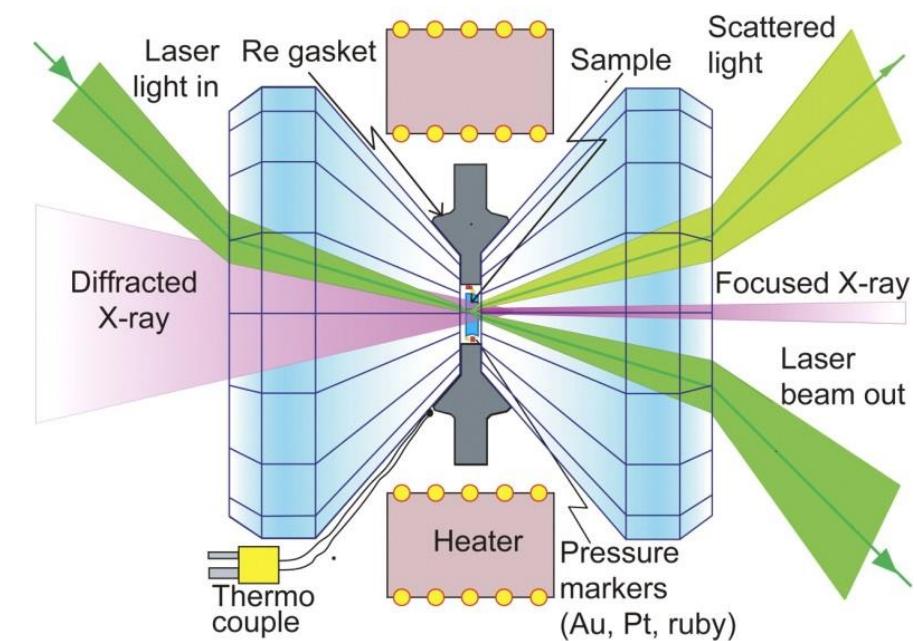
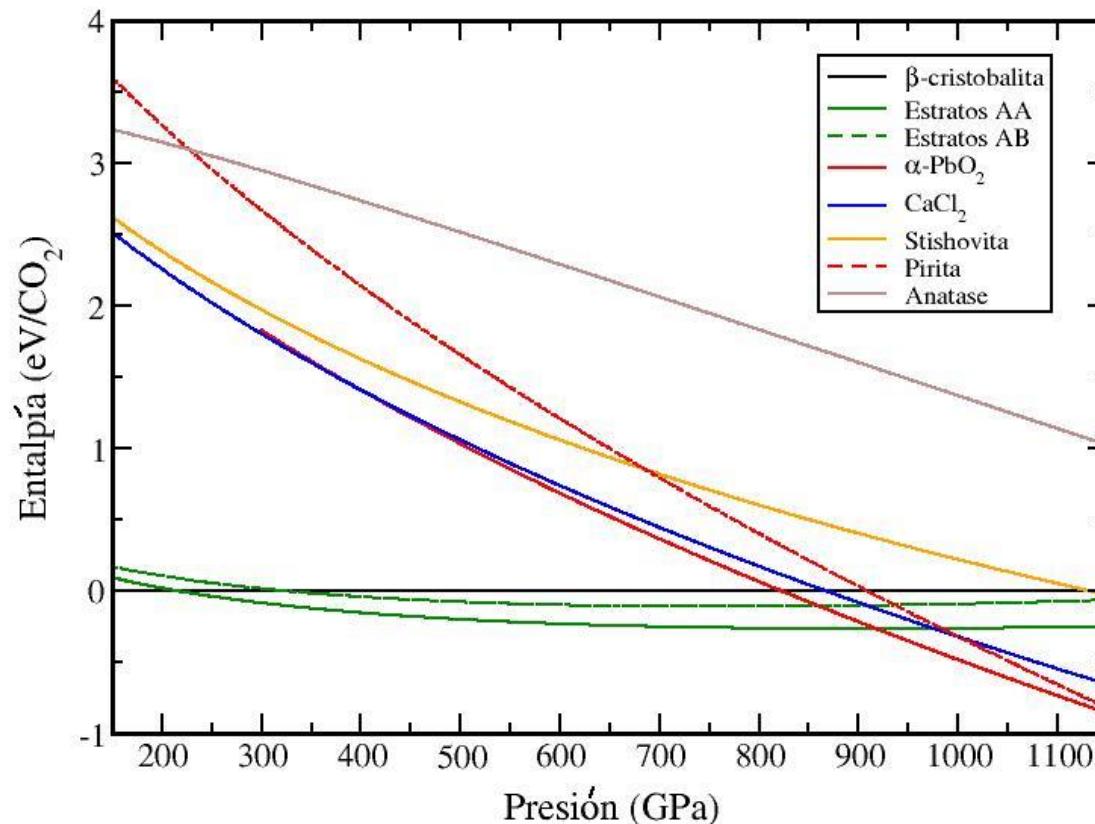
At NIF: Shockwave compression assisted by high-power lasers

Introduction

OUR PREVIOUS WORK WITH, CO₂, OXYGEN AND FLUORINE ASSUMED VERY AMPLE REGIONS OF STABILITY FOR THE EXISTENCE OF SOLID PHASES...

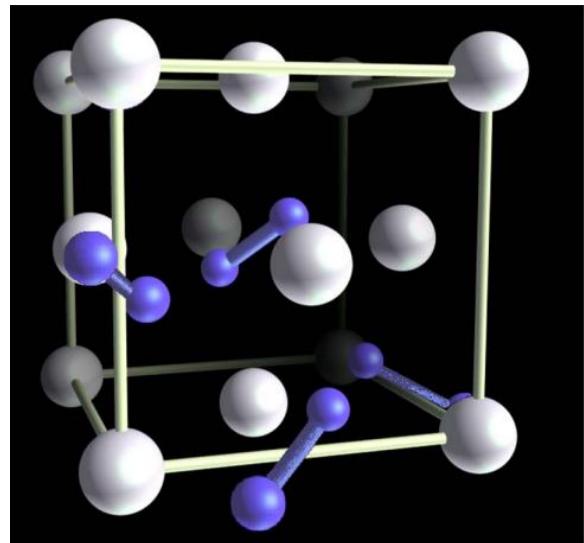
Previous work: Assuming
low temperature as the
same as zero temperature

Stability comparisons AT T=0K



Source: M.-S. Lee, J. A. Montoya and S. Scandolo, PRB **79**, 144102 (2009).

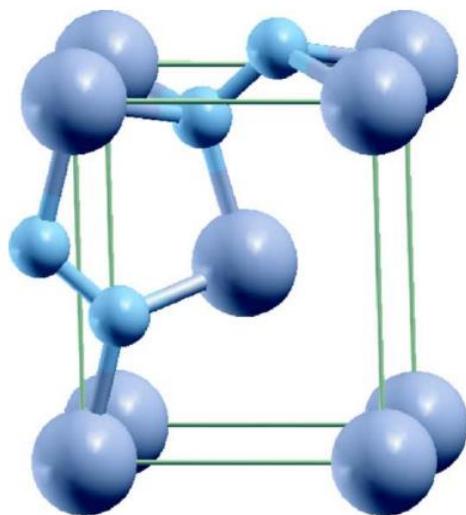
Previous work on structural prediction



PtN₂

Raman Spectra

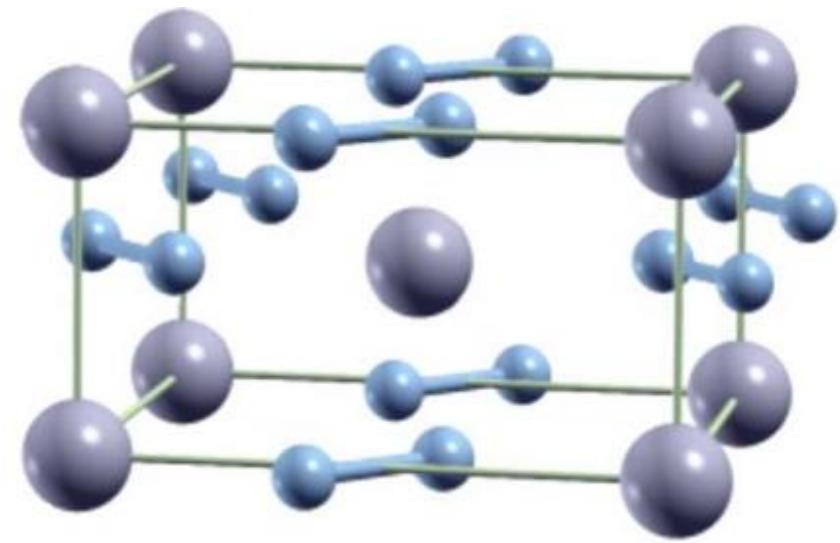
PRB 73, 153102 (2006)



OsN₂

X-Ray Diffraction

Appl. Phys. Lett. 90, 011909
2007

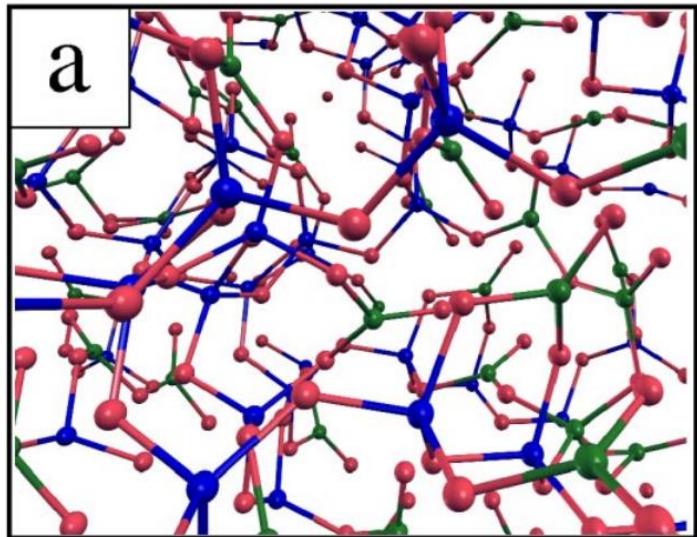


OsN₂

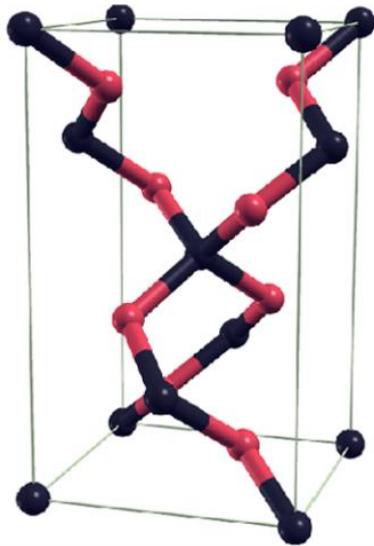
Tc

PRB 77, 092504 2008

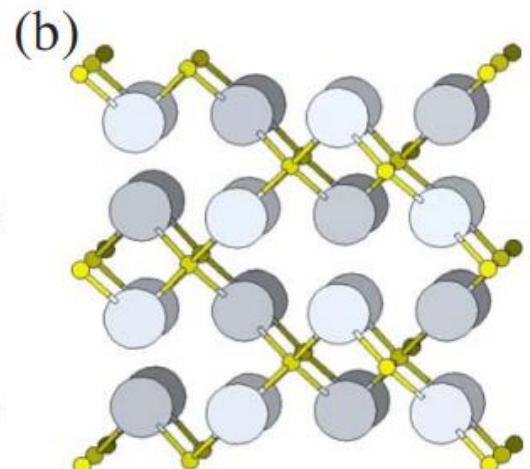
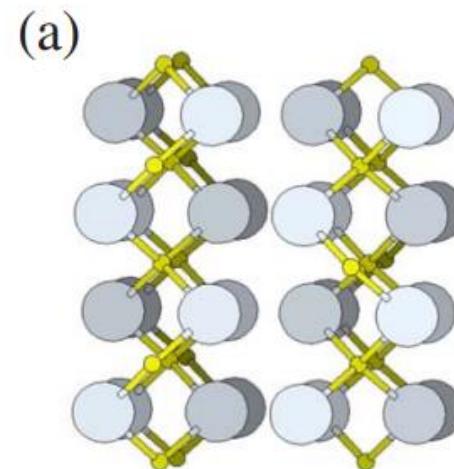
Previous work on structural prediction



IR and Raman Spectra
PRL 100, 163002 (2008)

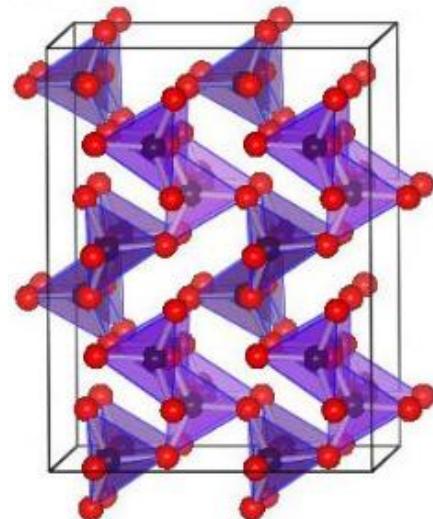


Raman Spectra
PRL 100, 163002 (2008)



CO₂
Raman Spectra
PRB 79, 144102 (2009)

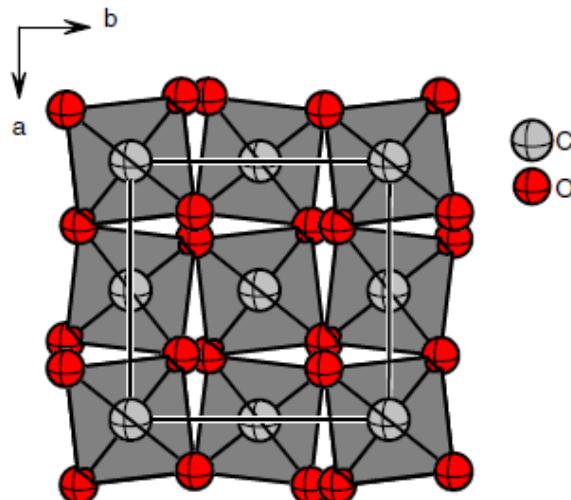
Previous work on structural prediction



CO₂

X-Ray Diffraction and Raman Spectra

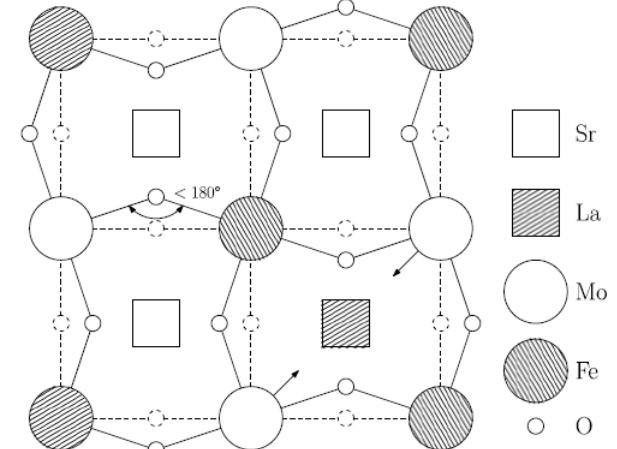
PNAS 106 (15), 6077 (2009)



CO₂-Phase V

Collapsed-cristobalite
IR + Raman Spectra

PNAS 109 (14), 5176 (2012)



Disordered double-perovskite

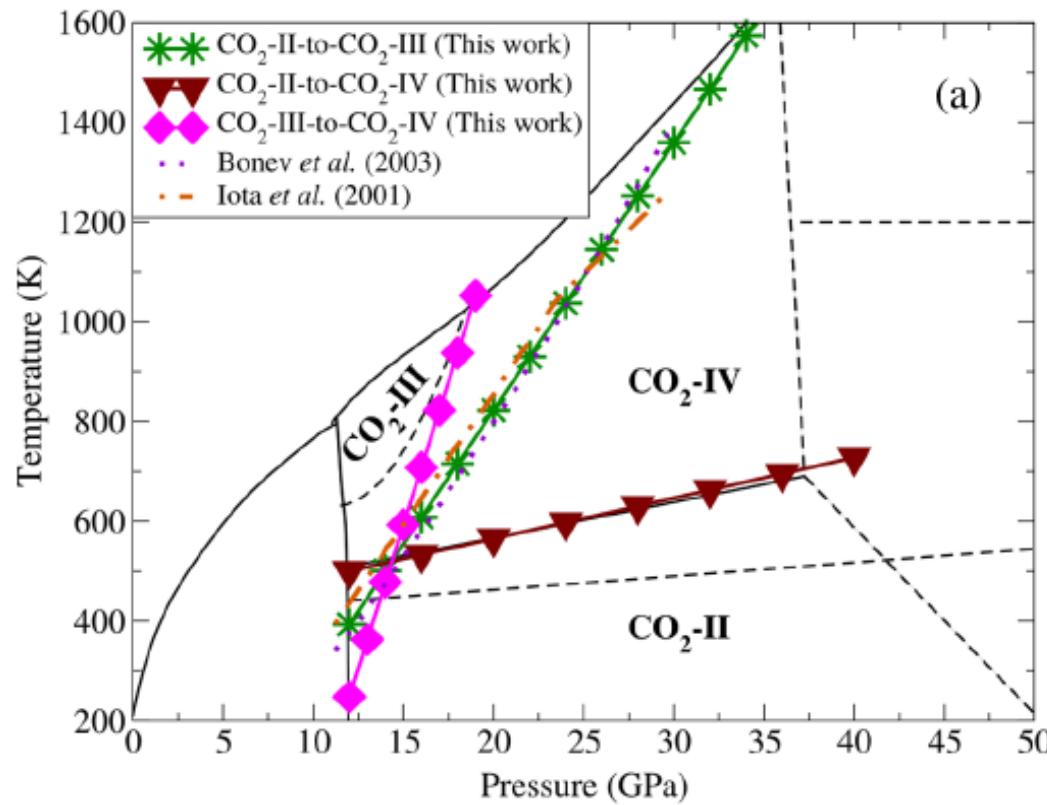
$\text{Sr}_{2-y}\text{La}_y\text{FeMoO}_6$

Composition analysis

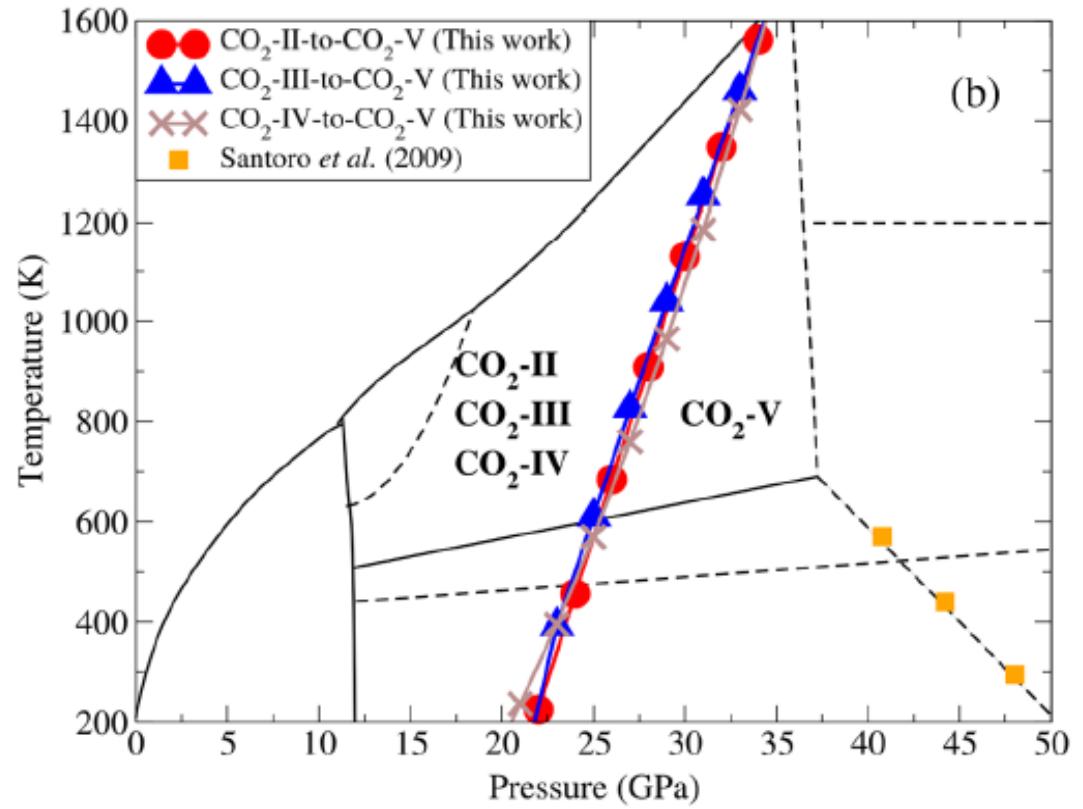
JMMM 495, 165877 (2020)

Previous work: Including
finite temperature effects
in energy comparisons

Stability comparisons when the melting curve is known



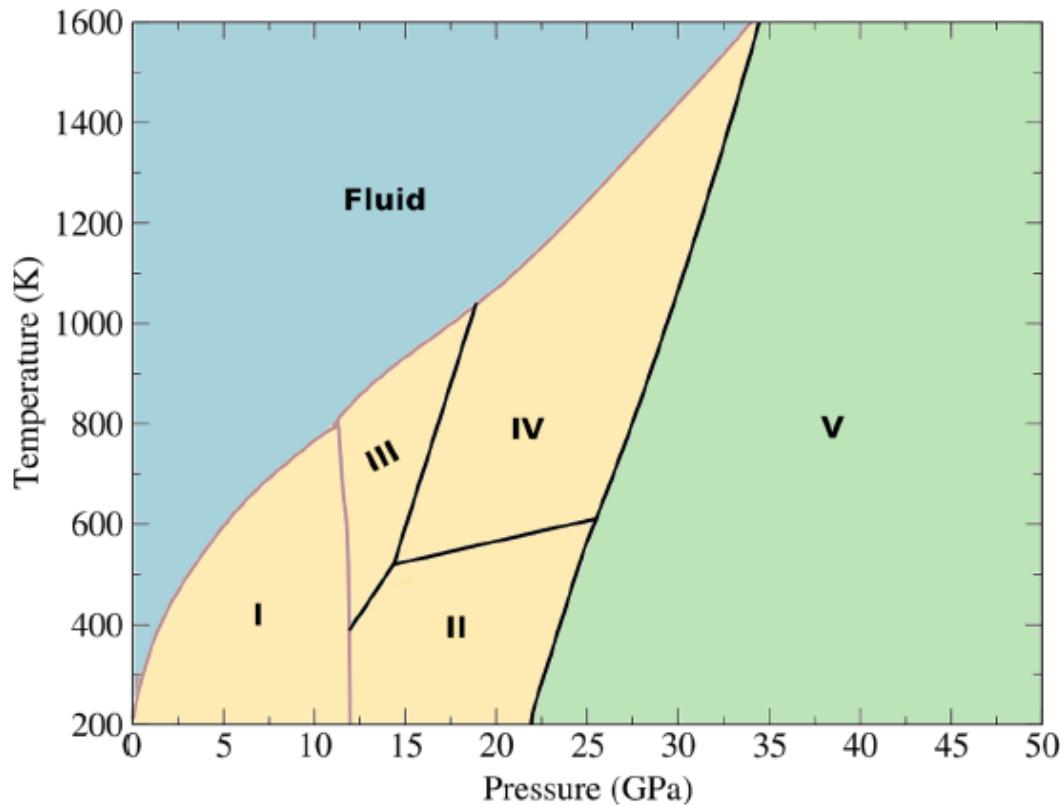
(a)



(b)

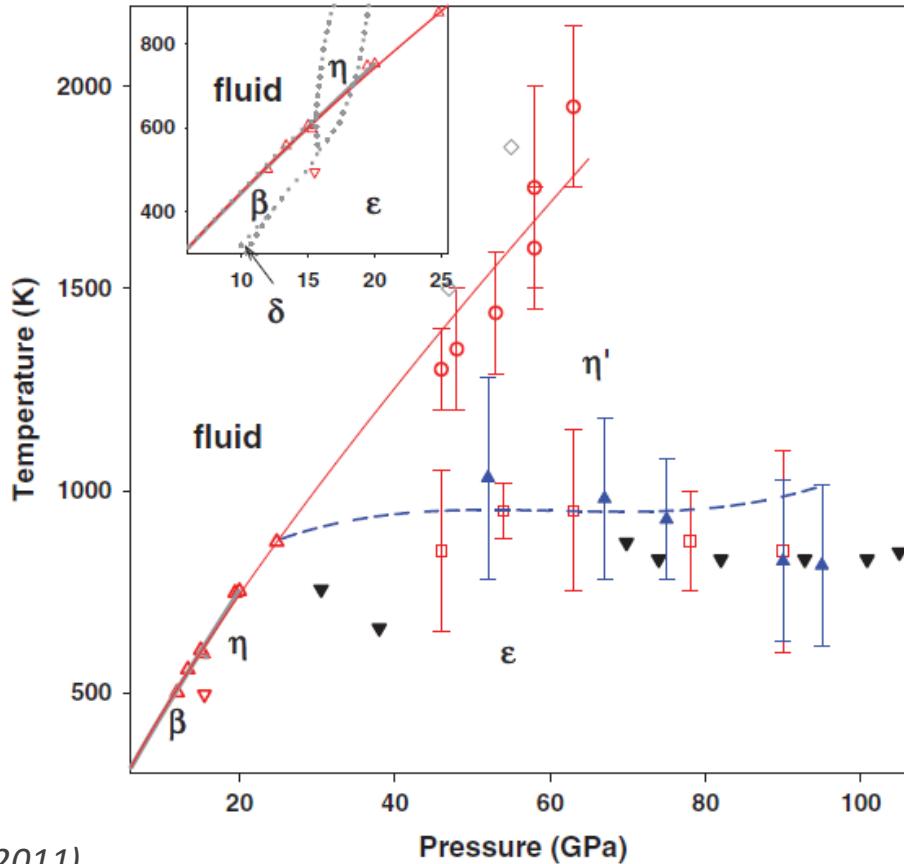
Source: PRL 124, 095701 (2020)

Stability comparisons when the melting curve is known



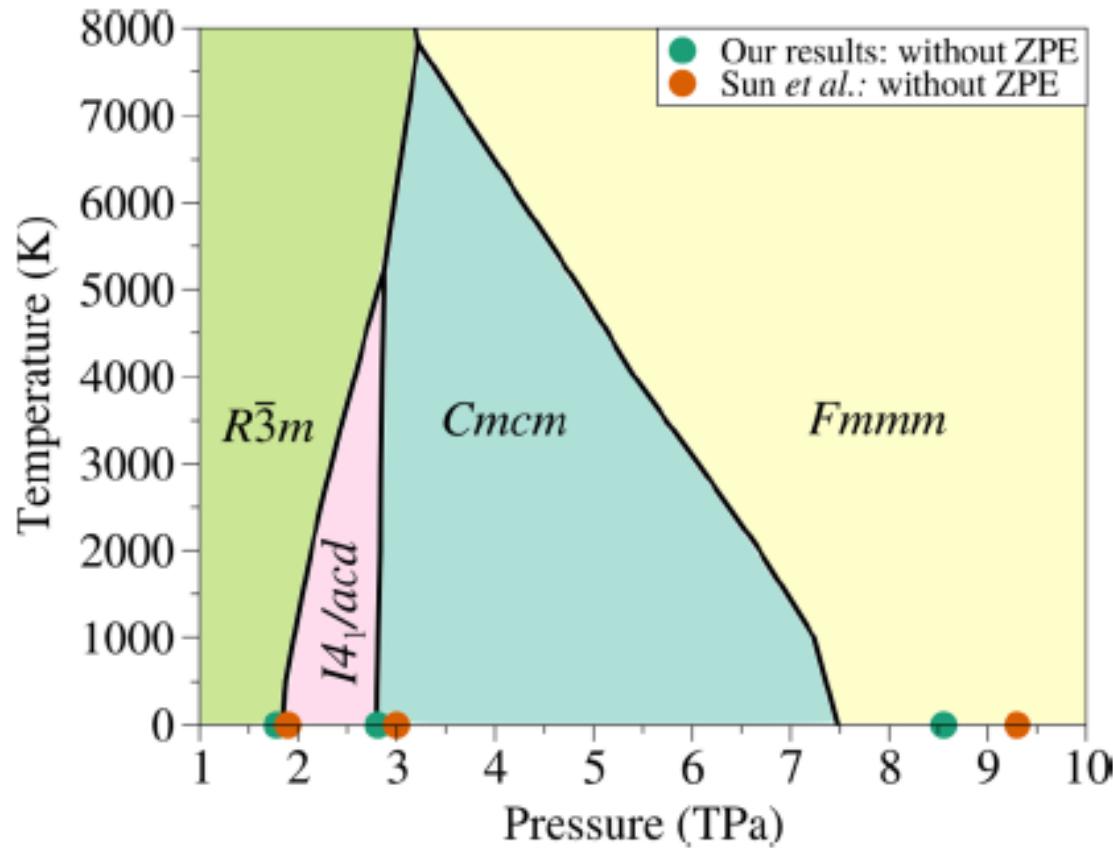
Source: PRL 124, 095701 (2020)

Stability comparisons when the melting curve is extrapolated



Source: J. Chem. Phys. 135, 084512 (2011)

Stability comparisons when the melting curve is extrapolated



Source: PRB 98, 094103 (2018)

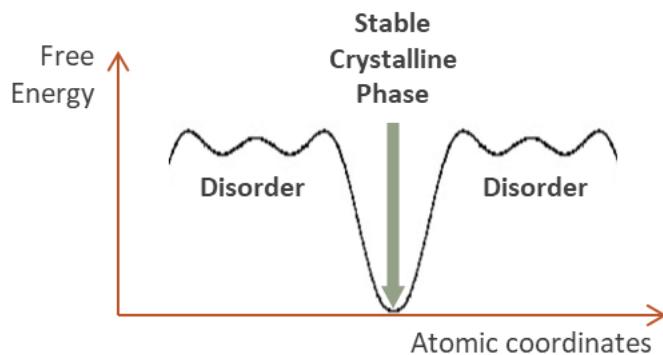


Melting Curves and Limitations for Precise Calculations

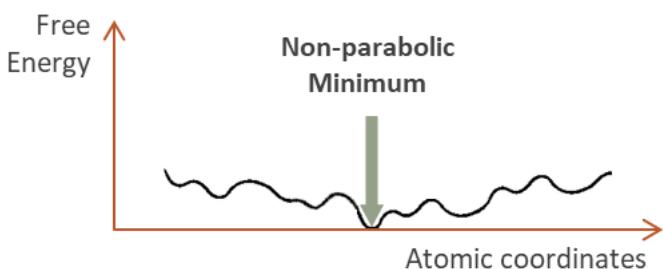
MELTING HYPOTHESES AND RARE EVENTS

Melting: two paradigms

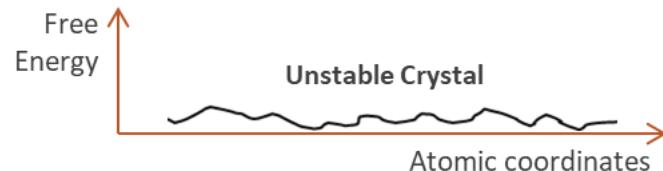
CATASTROPHE



$T = 0 \text{ K}$

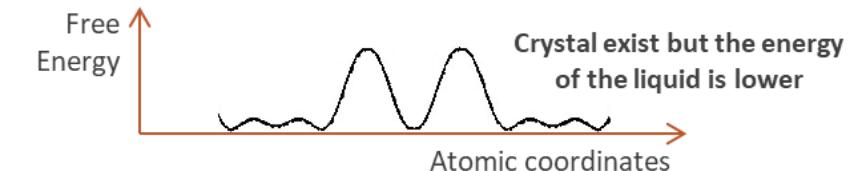
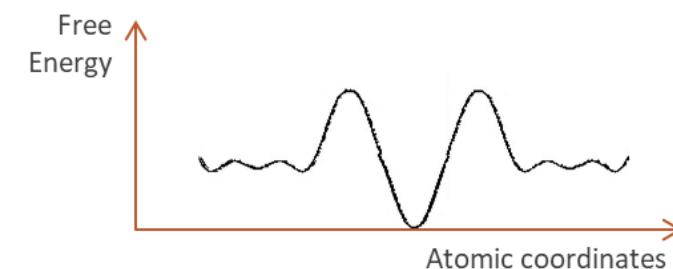
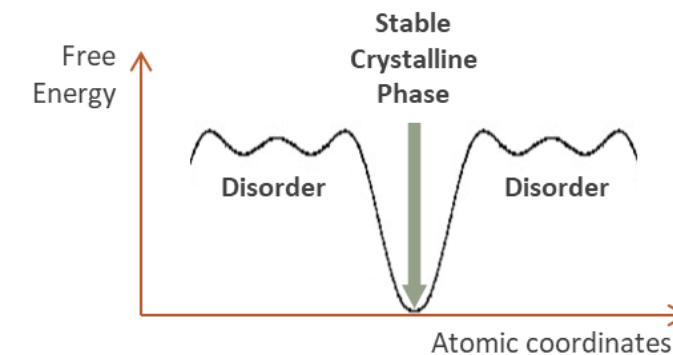


$T = T_m / 2$



$T = T_m$

NUCLEATION



Quasi- Harmonic Approximation

ASSUME THERE IS NO CATASTROPHE

Quasi-Harmonic Approximation

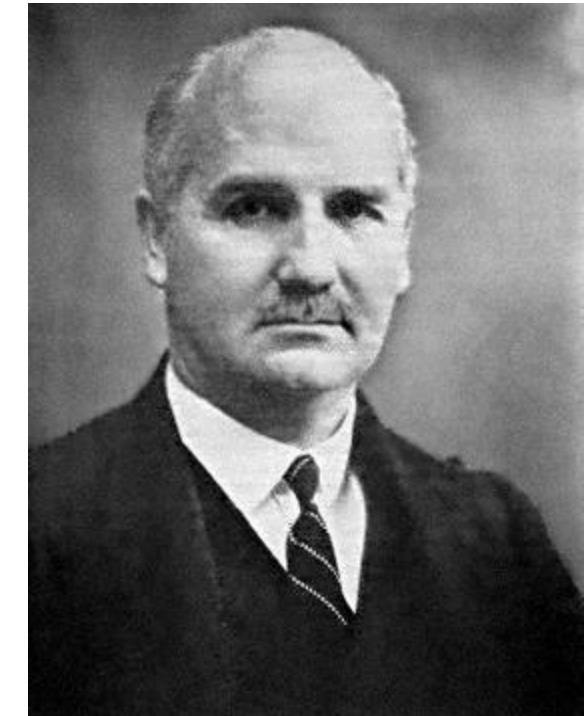
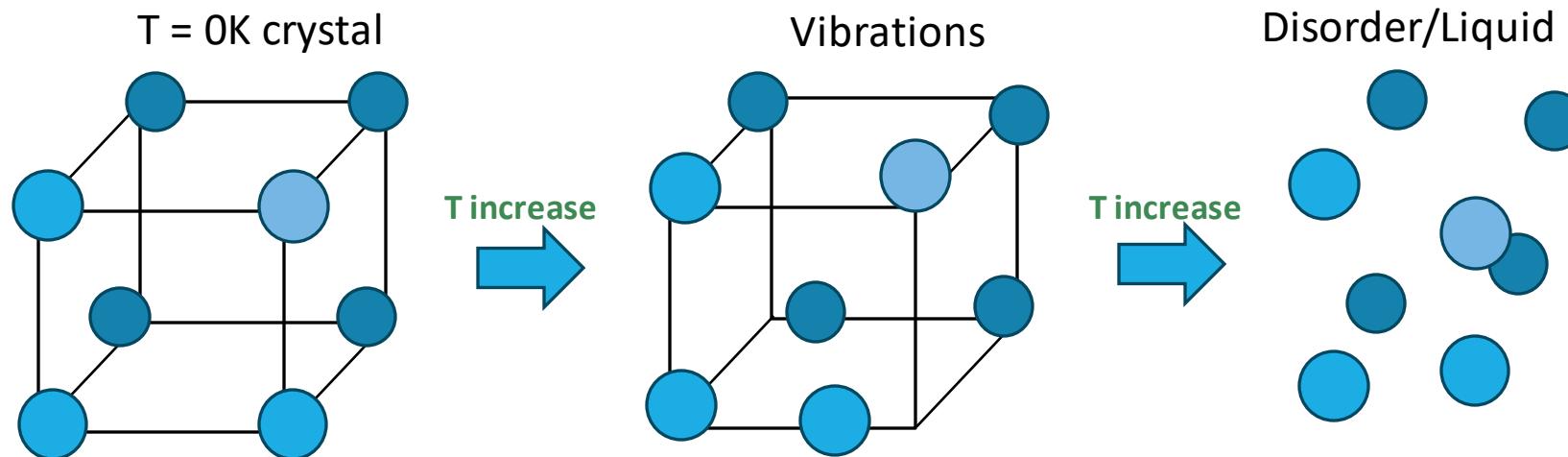
- In the Quasi-Harmonic Approximation (QHA) the anharmonicity is considered as a weak effect and the atomic forces and the frequencies are renormalized by taking only thermal expansion into account.
- In the QHA, the crystal free energy is determined via the regular harmonic expression, but constraining it (generally) to the volume:

$$F(V, T) = U_0(V) + \frac{1}{2} \sum_{\mathbf{q}} \hbar\omega(\mathbf{q}|V) + k_B T \sum_{\mathbf{q}} \ln[1 - \exp(-\hbar\omega(\mathbf{q}|V)/k_B T)]$$

Lindemann's Criteria

ENOUGH MOTION TO SCAPE

Frederick Alexander Lindemann's IDEA

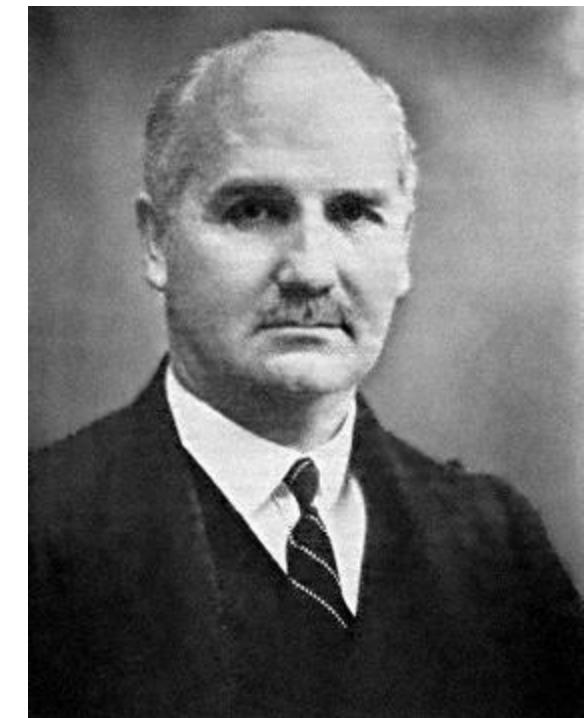


Frederick Alexander Lindemann's IDEA

Über die Berechnung molekularer Eigenfrequenzen¹).

Von F. A. Lindemann.

$$\eta = \frac{\langle \delta R_i^2 \rangle}{R_0^2} = \sum_{\mathbf{q},j} \frac{\langle E_{\mathbf{q},j} \rangle}{m n R_0^2 \omega_{\mathbf{q},j}^2} \quad \eta_m = \frac{k T_m}{m n R_0^2} \sum_{\mathbf{q},j} \omega_{\mathbf{q},j}^{-2}$$



On Lindemann's Melting Criterion

By

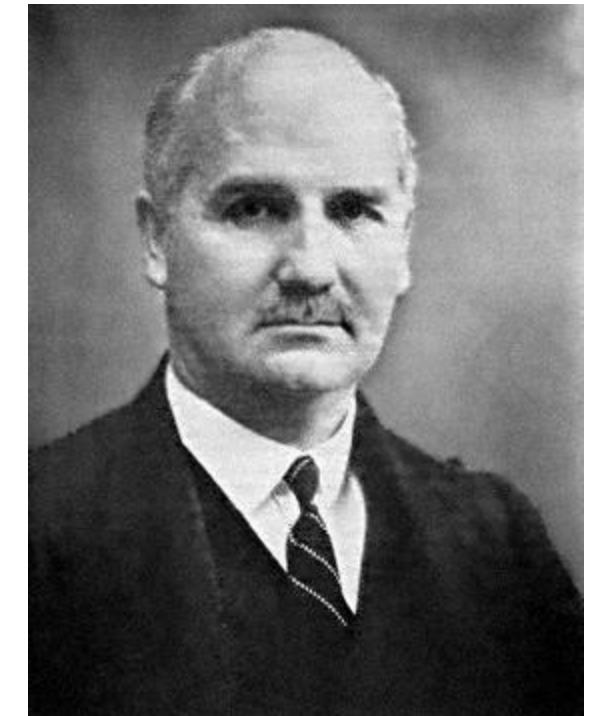
S. PAL and P. K. SHARMA

Frederick Alexander Lindemann's IDEA

Über die Berechnung molekularer Eigenfrequenzen¹).

Von F. A. Lindemann.

$$\eta = \frac{\langle \delta R_i^2 \rangle}{R_0^2} = \sum_{\mathbf{q},j} \frac{\langle E_{\mathbf{q},j} \rangle}{m n R_0^2 \omega_{\mathbf{q},j}^2} \quad \eta_m = \frac{k T_m}{m n R_0^2} \sum_{\mathbf{q},j} \omega_{\mathbf{q},j}^{-2}$$



On Lindemann's Melting Criterion

By

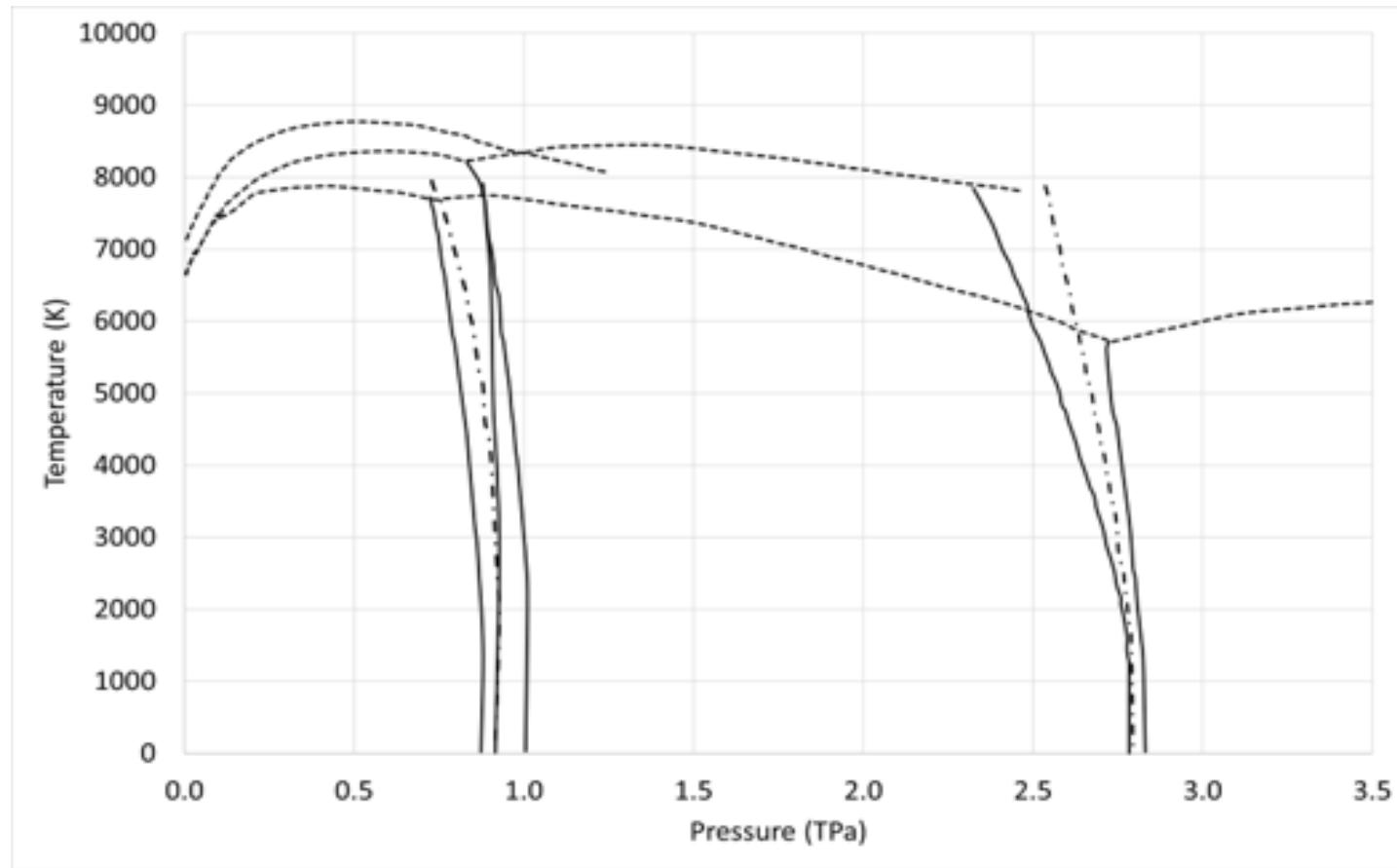
S. PAL and P. K. SHARMA



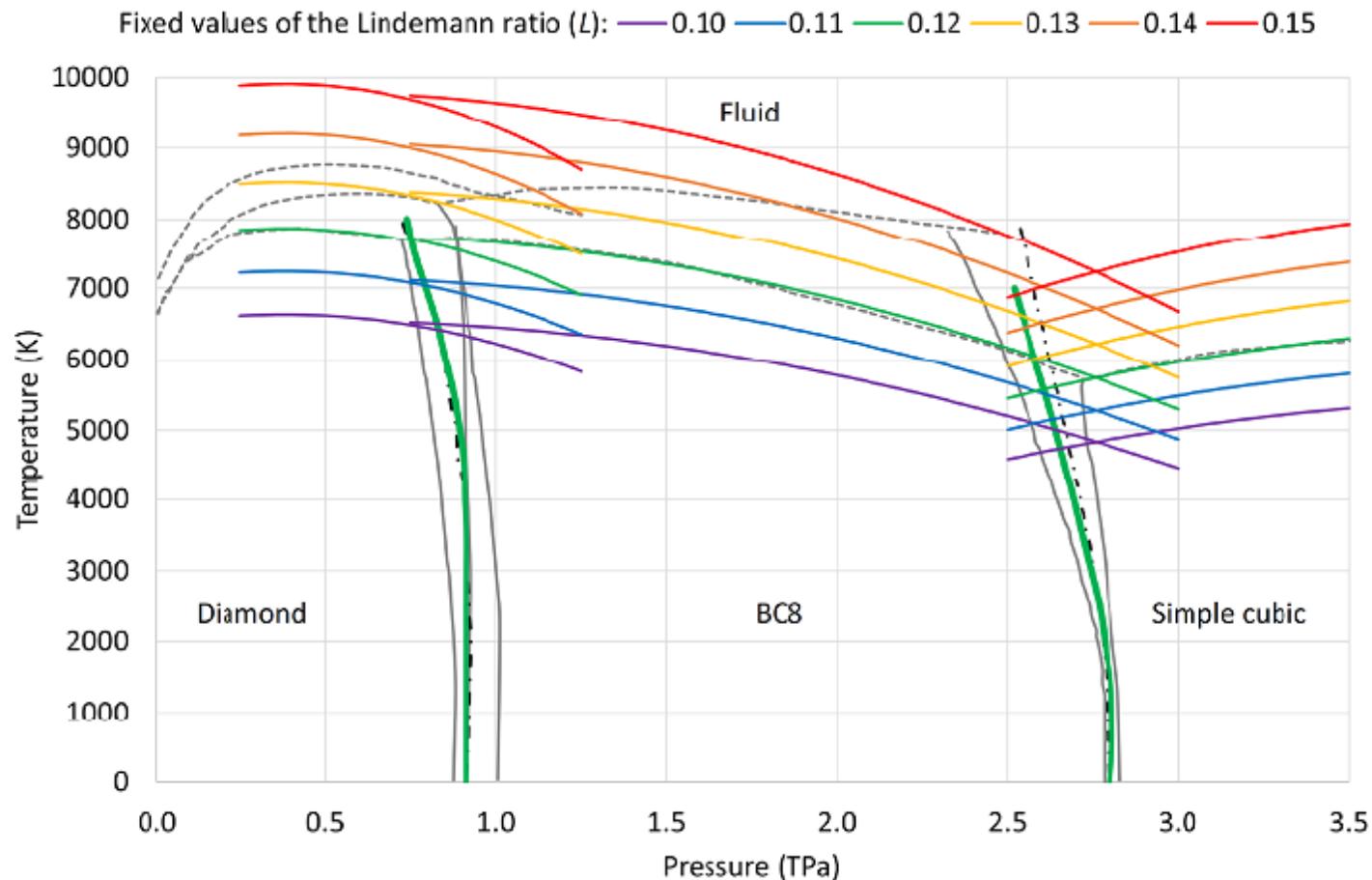
Identifying Melting Conditions on Carbon Phases

FROM DIAMOND TO SIMPLE CUBIC

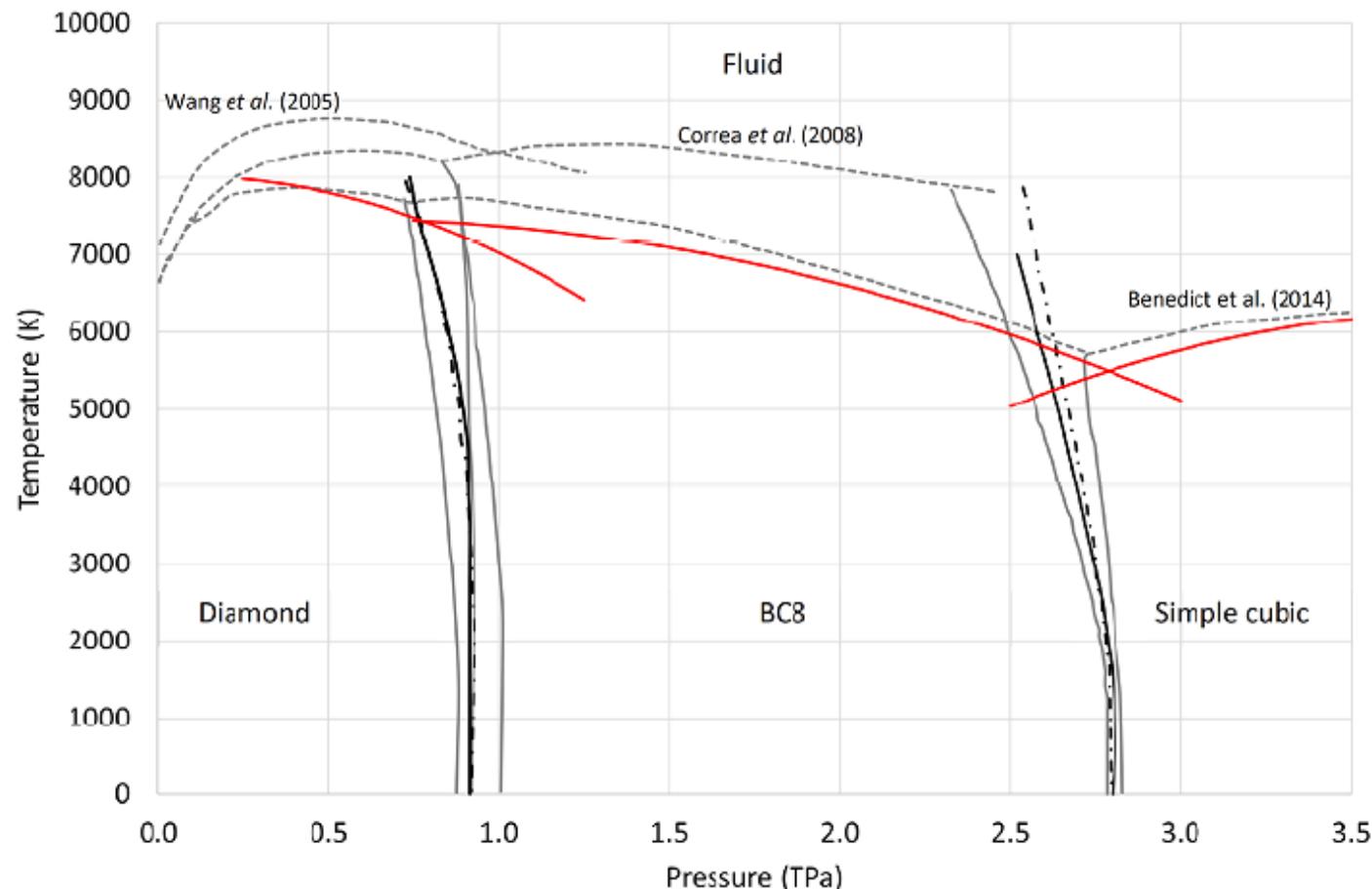
Carbon's Phase Diagram



Carbon's Phase Diagram



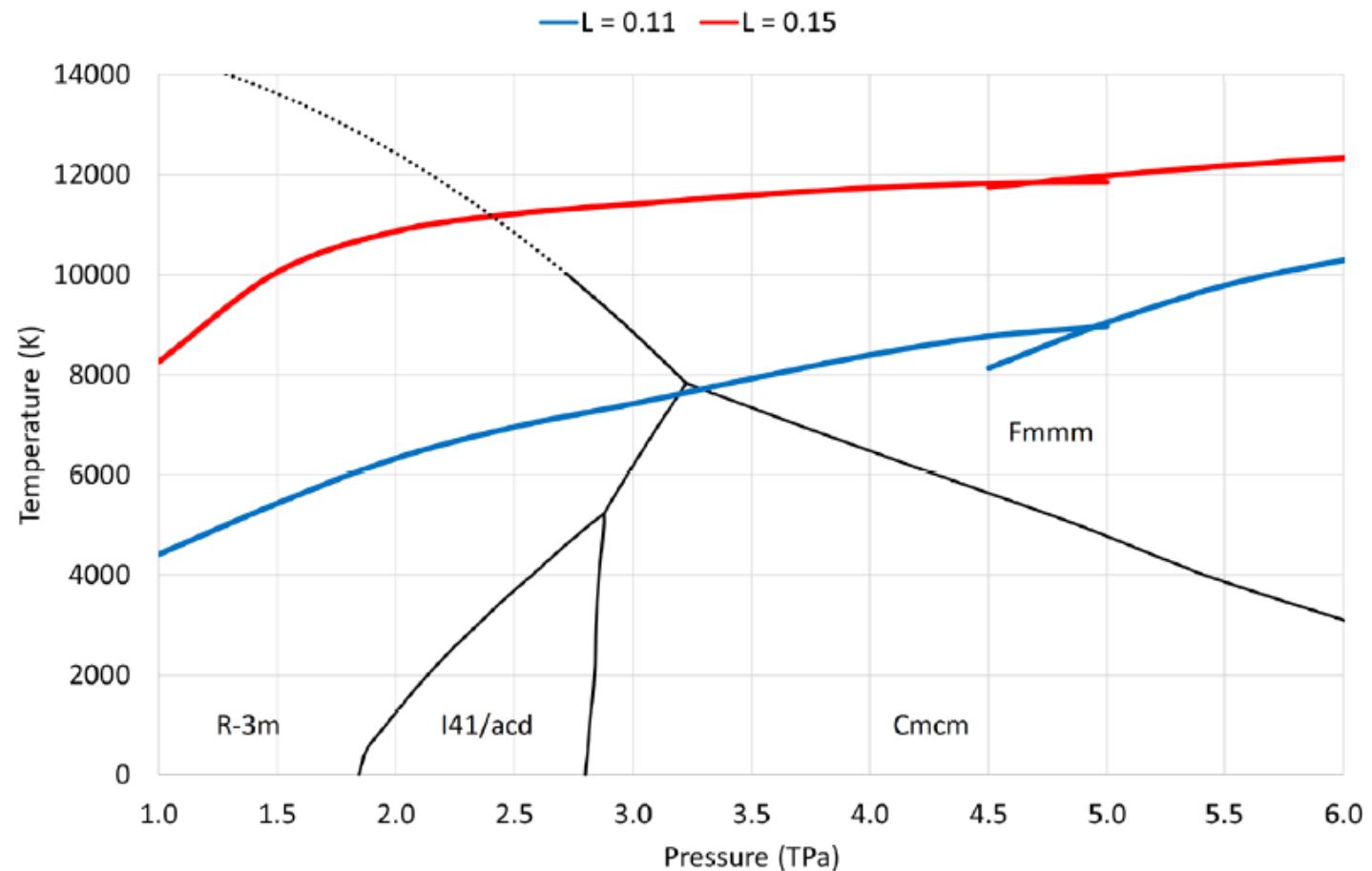
Carbon's Phase Diagram



Applicability Beyond Carbon

OXYGEN AND FLUORINE

Oxygen's Melting Curve



How it's done

Manual Approximation

Characterization and finite temperature contribution to a pressurized system

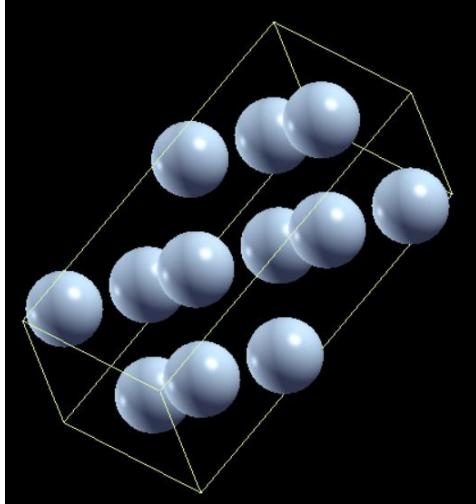
- System: Fluorine
- Specifications: Cmca 8 atoms/cell; Pressure: 3.5 TPa



Manual Approximation Ecut Convergence

```
#!/bin/bash
#SBATCH --job-name=Ecut-Ref
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=20
#SBATCH --time=72:00:00
#SBATCH --partition=normal

#Selecting module
module purge
module load QuantumExpresso/6.7.0
```



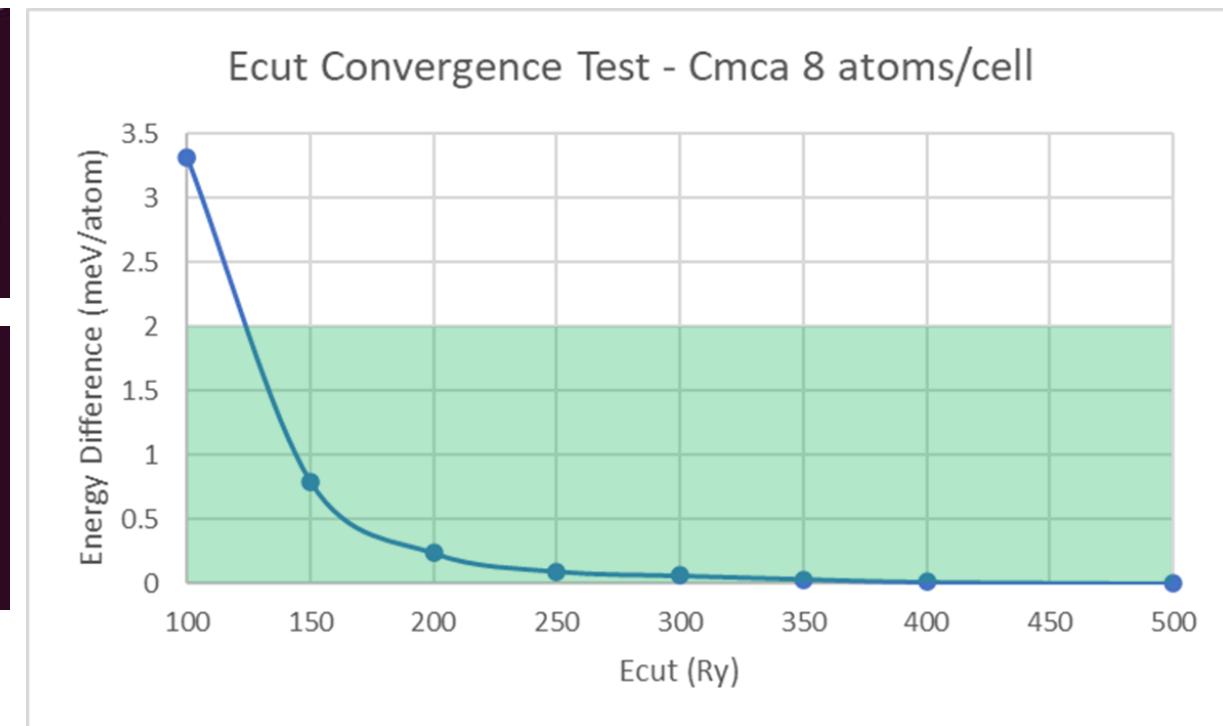
```
for ECUT in 100 150 200 250 300 350 400 500
do
    cat > Ecut-$ECUT-5.0-TPa-64.in << FINAL
    &control
        title = 'F2_64',
        calculation = 'scf',
        restart_mode = 'from_scratch',
        verbosity = 'minimal',
        disk_io = 'none',
        wf_collect = .false.,
        nstep = 100,
        prefix = 'F2_64',
        pseudo_dir = '$PSEUDO_DIR',
        outdir = '$SCRATCH_DIR',
        etot_conv_thr = 1.0d-8,
        forc_conv_thr = 1.0d-3,
        tstress = .true.,
        tprnfor = .true.
    /
    &system
        ibrav = 8,
        celldm(1) = 3.487367168,
        celldm(2) = 0.999991125,
        celldm(3) = 2.327660345,
        nat = 8,
        ntyp = 1,
        ecutwfc = $ECUT,
        ecutrho = $((ECUT*8)),
        occupations = 'smearing',
        smearing = 'fermi-dirac',
        degauss = 3.167d-3
    /
&electrons
electron_maxstep = 500,
conv_thr = 1.0d-9,
mixing_mode = 'TF',
mixing_beta = 0.55,
diagonalization = 'david',
diago_david_ndim = 4
/
ATOMIC_SPECIES
F 18.9984 F.pbe-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
F 0.0000 -0.2500 -0.1250
F 0.0000 0.7500 0.3750
F 0.0000 0.2500 0.6250
F 0.0000 0.2500 0.1250
F 0.5000 0.2500 -0.1250
F 0.5000 1.2500 0.3750
F 0.5000 0.7500 0.6250
F 0.5000 0.7500 0.1250
K_POINTS {automatic}
8 8 4 0 0 0
FINAL
#####
mpirun pw.x -inp Ecut-$ECUT-5.0-TPa-64.in > Ecut-$ECUT-5.0-TPa-64.out
#####
done
```

Manual Approximation Ecut Convergence

Cmca 8 atoms - Ecut Results:

```
(base) max@qmobile:~/Fluor/02-References$ grep ! Ref-Ecut/Ecut-*.-64.out
Ref-Ecut/Ecut-100-5.0-TPa-64.out:! total energy      = -456.54965179 Ry
Ref-Ecut/Ecut-150-5.0-TPa-64.out:! total energy      = -456.55113345 Ry
Ref-Ecut/Ecut-200-5.0-TPa-64.out:! total energy      = -456.55145991 Ry
Ref-Ecut/Ecut-250-5.0-TPa-64.out:! total energy      = -456.55154344 Ry
Ref-Ecut/Ecut-300-5.0-TPa-64.out:! total energy      = -456.55156261 Ry
Ref-Ecut/Ecut-350-5.0-TPa-64.out:! total energy      = -456.55157895 Ry
Ref-Ecut/Ecut-400-5.0-TPa-64.out:! total energy      = -456.55159149 Ry
Ref-Ecut/Ecut-500-5.0-TPa-64.out:! total energy      = -456.55159973 Ry
```

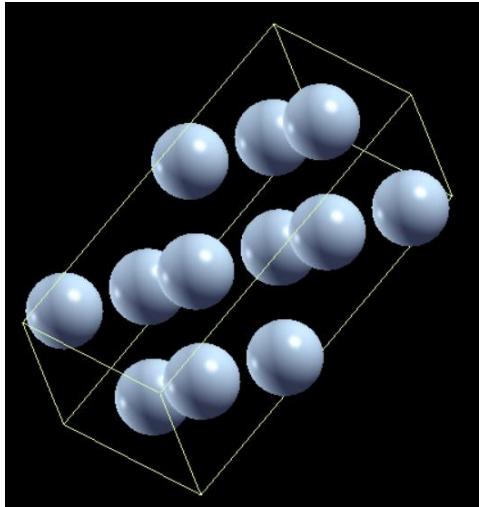
```
(base) max@qmobile:~/Fluor/02-References$ grep "PWSCF      :" Ref-Ecut/Ecut-*.-64.out
Ref-Ecut/Ecut-100-5.0-TPa-64.out: PWSCF      : 36.09s CPU    37.44s WALL
Ref-Ecut/Ecut-150-5.0-TPa-64.out: PWSCF      : 49.42s CPU    50.87s WALL
Ref-Ecut/Ecut-200-5.0-TPa-64.out: PWSCF      : 1m 0.34s CPU   1m 4.11s WALL
Ref-Ecut/Ecut-250-5.0-TPa-64.out: PWSCF      : 1m23.57s CPU   1m25.35s WALL
Ref-Ecut/Ecut-300-5.0-TPa-64.out: PWSCF      : 1m44.55s CPU   1m46.33s WALL
Ref-Ecut/Ecut-350-5.0-TPa-64.out: PWSCF      : 2m10.31s CPU   2m12.16s WALL
Ref-Ecut/Ecut-400-5.0-TPa-64.out: PWSCF      : 2m33.80s CPU   2m38.68s WALL
Ref-Ecut/Ecut-500-5.0-TPa-64.out: PWSCF      : 3m19.56s CPU   3m21.90s WALL
```



Manual Approximation K Points Convergence

```
#!/bin/bash
#SBATCH --job-name=KPts-Ref
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=20
#SBATCH --time=72:00:00
#SBATCH --partition=normal

#Selecting module
module purge
module load QuantumExpresso/6.7.0
```



```
for KPTS in 1 2 3 4 5 REF
do
    cat > KPts-$KPTS-5.0-TPa-64.in << FINAL
    &control
        title = 'F2_64',
        calculation = 'scf',
        restart_mode = 'from_scratch',
        verbosity = 'minimal',
        disk_io = 'none',
        wf_collect = .false.,
        nstep = 100,
        prefix = 'F2_64',
        pseudo_dir = '$PSEUDO_DIR',
        outdir = '$SCRATCH_DIR',
        etot_conv_thr = 1.0d-8,
        forc_conv_thr = 1.0d-3,
        tstress = .true.,
        tprnfor = .true.
    /
    &system
        ibrav = 8,
        celldm(1) = 3.487367168,
        celldm(2) = 0.999991125,
        celldm(3) = 2.327660345,
        nat = 8,
        ntyp = 1,
        ecutwfc = 200,
        ecutrho = 1600,
        occupations = 'smearing',
        smearing = 'fermi-dirac',
        degauss = 3.167d-3
    /
```

```
&electrons
electron_maxstep = 500,
conv_thr = 1.0d-9,
mixing_mode = 'TF',
mixing_beta = 0.55,
diagonalization = 'david',
diago_david_ndim = 4
/
ATOMIC_SPECIES
F 18.9984 F.pbe-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
F 0.0000 -0.2500 -0.1250
F 0.0000 0.7500 0.3750
F 0.0000 0.2500 0.6250
F 0.0000 0.2500 0.1250
F 0.5000 0.2500 -0.1250
F 0.5000 1.2500 0.3750
F 0.5000 0.7500 0.6250
F 0.5000 0.7500 0.1250
K_POINTS {automatic}
FINAL

case $KPTS in
1) echo " 4   4   2   0 0 0" >> KPts-$KPTS-5.0-TPa-64.in ;;
2) echo " 8   8   4   0 0 0" >> KPts-$KPTS-5.0-TPa-64.in ;;
3) echo " 12  12  6   0 0 0" >> KPts-$KPTS-5.0-TPa-64.in ;;
4) echo " 16  16  8   0 0 0" >> KPts-$KPTS-5.0-TPa-64.in ;;
5) echo " 20  20  10  0 0 0" >> KPts-$KPTS-5.0-TPa-64.in ;;
REF) echo " 28  28  14  0 0 0" >> KPts-$KPTS-5.0-TPa-64.in ;;
esac

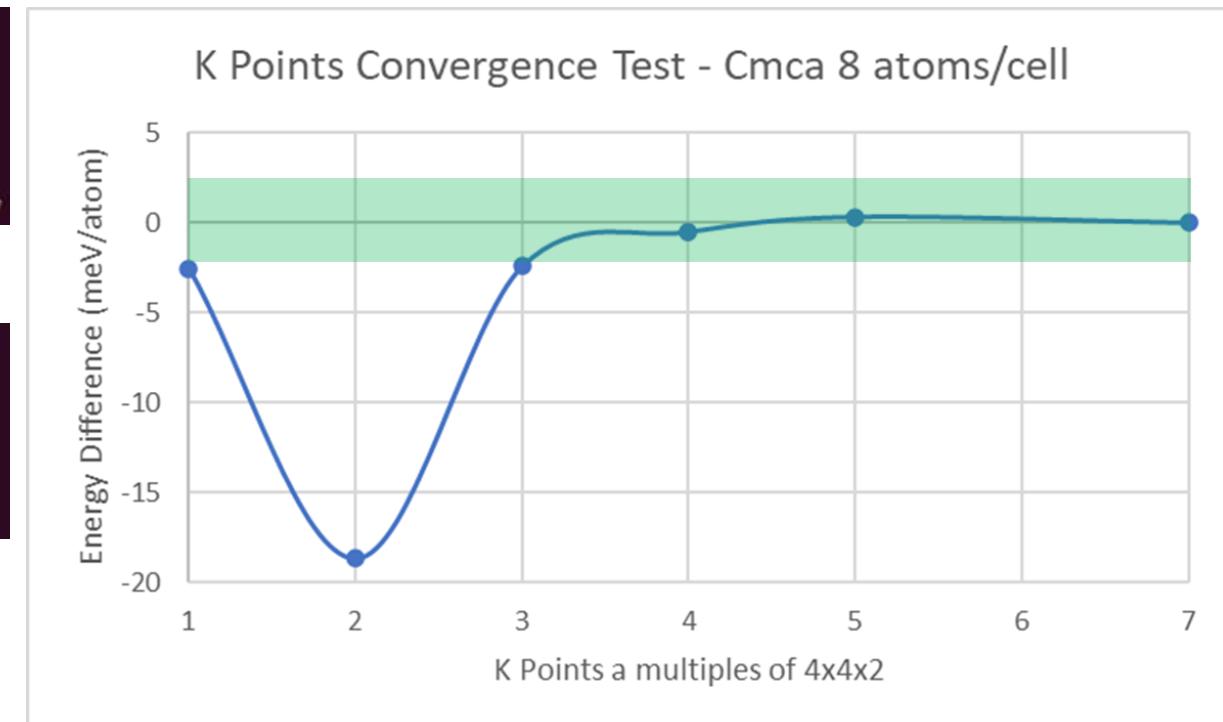
#####
mpirun pw.x -inp KPts-$KPTS-5.0-TPa-64.in > KPts-$KPTS-5.0-TPa-64.out
#####
done
```

Manual Approximation K Points Convergence

Cmca 8 atoms - K Points Results:

```
(base) max@qmobile:~/Fluor/02-References$ grep ! Ref-KPts/KPts-* -64.out
Ref-KPts/KPts-1-5.0-TPa-64.out:!    total energy      =   -456.54198014 Ry
Ref-KPts/KPts-2-5.0-TPa-64.out:!    total energy      =   -456.55145991 Ry
Ref-KPts/KPts-3-5.0-TPa-64.out:!    total energy      =   -456.54190863 Ry
Ref-KPts/KPts-4-5.0-TPa-64.out:!    total energy      =   -456.54078559 Ry
Ref-KPts/KPts-5-5.0-TPa-64.out:!    total energy      =   -456.54029275 Ry
Ref-KPts/KPts-REF-5.0-TPa-64.out:!  total energy      =   -456.54048366 Ry
```

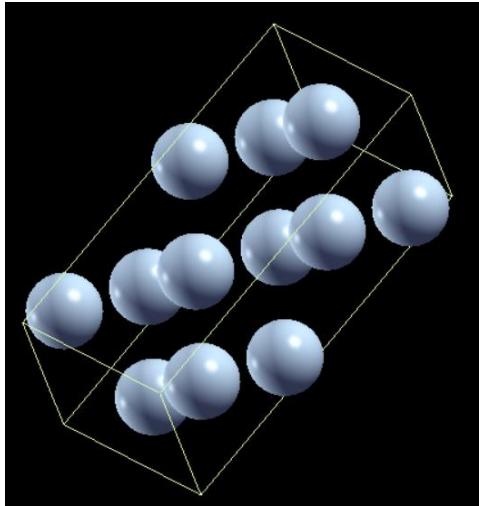
```
(base) max@qmobile:~/Fluor/02-References$ grep "PWSCF      :" Ref-KPts/KPts-* -64.out
Ref-KPts/KPts-1-5.0-TPa-64.out:  PWSCF      :  14.92s CPU  15.32s WALL
Ref-KPts/KPts-2-5.0-TPa-64.out:  PWSCF      : 1m 0.24s CPU  1m 1.78s WALL
Ref-KPts/KPts-3-5.0-TPa-64.out:  PWSCF      : 3m18.85s CPU  3m30.02s WALL
Ref-KPts/KPts-4-5.0-TPa-64.out:  PWSCF      : 6m17.58s CPU  6m26.42s WALL
Ref-KPts/KPts-5-5.0-TPa-64.out:  PWSCF      : 11m59.01s CPU  12m16.83s WALL
Ref-KPts/KPts-REF-5.0-TPa-64.out: PWSCF      : 33m12.86s CPU  34m34.25s WALL
```



Manual Approximation VC Relax

```
#!/bin/bash
#SBATCH --job-name=VCRelx-Ref
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=20
#SBATCH --time=72:00:00
#SBATCH --partition=normal

#Selecting module
module purge
module load QuantumExpresso/6.7.0
```



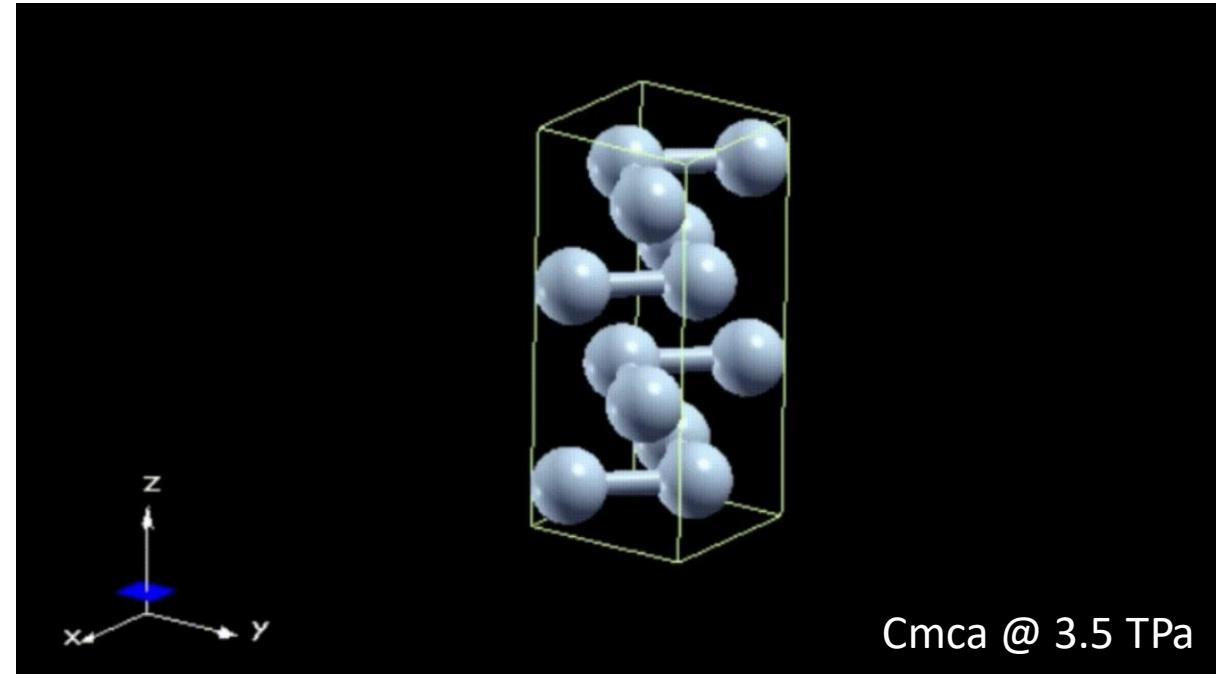
```
for P in 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.0
do
    PRESSURE=`echo "$P*10000" | bc`
    cat > VC-Relax-$P-TPa-64.in << FINAL
    &control
        title = 'F2_64',
        calculation = 'vc-relax',
        restart_mode = 'from_scratch',
        verbosity = 'minimal',
        disk_io = 'none',
        wf_collect = .false.,
        nstep = 100,
        prefix = 'F2_64',
        pseudo_dir = '$PSEUDO_DIR',
        outdir = '$SCRATCH_DIR',
        etot_conv_thr = 1.0d-8,
        forc_conv_thr = 1.0d-3,
        tstress = .true.,
        tprnfor = .true.
    /
    &system
        ibrav = 8,
        celldm(1) = 3.487367168,
        celldm(2) = 0.999991125,
        celldm(3) = 2.327660345,
        nat = 8,
        ntyp = 1,
        ecutwfc = 200,
        ecutrho = 1600,
        occupations = 'smearing',
        smearing = 'fermi-dirac',
        degauss = 3.167d-3
    /
&electrons
electron_maxstep = 500,
conv_thr = 1.0d-9,
mixing_mode = 'TF',
mixing_beta = 0.55,
diagonalization = 'david',
diago_david_ndim = 4
/
&ions
ion_dynamics = 'bfgs',
upscale = 10.0d0,
trust_radius_ini = 5.0d-3,
trust_radius_max = 1.0d-1,
trust_radius_min = 1.0d-10
/
&cell
cell_dynamics = 'bfgs',
cell_factor = 1.4,
press = $PRESSURE,
press_conv_thr = 5
/
ATOMIC_SPECIES
F 18.9984 F.pbe-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
$AP1
$AP2
$AP3
$AP4
$AP5
$AP6
$AP7
$AP8
K_POINTS {automatic}
16 16 8 0 0 0
FINAL
```

Manual Approximation VC Relax

Cmca 8 atoms - VC Relax Results:

```
(base) max@qmobile:~/Fluor/02-References$ grep " bfgs converged" Ref-VCRelax/VC-Relax-*-TPa-64.out
Ref-VCRelax/VC-Relax-1.0-TPa-64.out:      bfgs converged in 35 scf cycles and 32 bfgs steps
Ref-VCRelax/VC-Relax-2.0-TPa-64.out:      bfgs converged in 27 scf cycles and 23 bfgs steps
Ref-VCRelax/VC-Relax-2.5-TPa-64.out:      bfgs converged in 34 scf cycles and 24 bfgs steps
Ref-VCRelax/VC-Relax-3.0-TPa-64.out:      bfgs converged in 29 scf cycles and 20 bfgs steps
Ref-VCRelax/VC-Relax-3.5-TPa-64.out:      bfgs converged in 31 scf cycles and 21 bfgs steps
Ref-VCRelax/VC-Relax-4.0-TPa-64.out:      bfgs converged in 24 scf cycles and 17 bfgs steps
Ref-VCRelax/VC-Relax-4.5-TPa-64.out:      bfgs converged in 22 scf cycles and 14 bfgs steps
Ref-VCRelax/VC-Relax-5.0-TPa-64.out:      bfgs converged in 25 scf cycles and 16 bfgs steps
```

```
(base) max@qmobile:~/Fluor/02-References$ grep "PWSCF"      :" Ref-VCRelax/VC-Relax-*-TPa-64.out
Ref-VCRelax/VC-Relax-1.0-TPa-64.out:      PWSCF      : 4h53m CPU      5h25m WALL
Ref-VCRelax/VC-Relax-2.0-TPa-64.out:      PWSCF      : 4h42m CPU      5h 6m WALL
Ref-VCRelax/VC-Relax-2.5-TPa-64.out:      PWSCF      : 7h32m CPU      8h 1m WALL
Ref-VCRelax/VC-Relax-3.0-TPa-64.out:      PWSCF      : 3h57m CPU      4h17m WALL
Ref-VCRelax/VC-Relax-3.5-TPa-64.out:      PWSCF      : 4h11m CPU      4h21m WALL
Ref-VCRelax/VC-Relax-4.0-TPa-64.out:      PWSCF      : 3h 8m CPU      3h14m WALL
Ref-VCRelax/VC-Relax-4.5-TPa-64.out:      PWSCF      : 2h34m CPU      2h40m WALL
Ref-VCRelax/VC-Relax-5.0-TPa-64.out:      PWSCF      : 2h26m CPU      2h33m WALL
```



Manual Approximation SCF

```
#!/bin/bash
#SBATCH --job-name=SCF-64
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=20
#SBATCH --time=72:00:00
#SBATCH --partition=normal

>Selecting module
module purge
module load QuantumExpresso/6.7.0
```

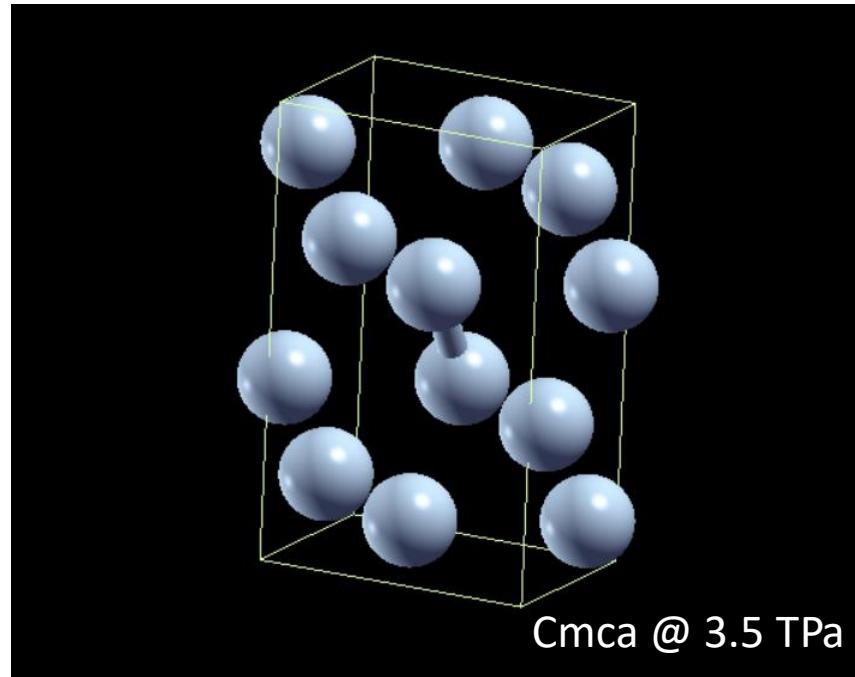
```
for P in 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.0
do
    case $P in
        1.0) CD1="5.458511313" ; CD2="0.682148644" ; CD3="1.587920458" ;;
        2.0) CD1="5.002520000" ; CD2="0.687178784" ; CD3="1.618575319" ;;
        2.5) CD1="4.857108946" ; CD2="0.689919396" ; CD3="1.626616347" ;;
        3.0) CD1="4.738531936" ; CD2="0.692780917" ; CD3="1.632513098" ;;
        3.5) CD1="4.638370980" ; CD2="0.695738171" ; CD3="1.636995269" ;;
        4.0) CD1="4.551472109" ; CD2="0.698822334" ; CD3="1.640522225" ;;
        4.5) CD1="4.474626078" ; CD2="0.702030761" ; CD3="1.643309651" ;;
        5.0) CD1="4.405840146" ; CD2="0.705255206" ; CD3="1.645590174" ;;
    esac
    cat > SCF-$P-TPa-64.in << FINAL
    &control
        title = 'F2_64',
        calculation = 'scf',
        restart_mode = 'from_scratch',
        verbosity = 'minimal',
        disk_io = 'none',
        wf_collect = .false.,
        nstep = 100,
        prefix = 'F2_64',
        pseudo_dir = '$PSEUDO_DIR',
        outdir = '$SCRATCH_DIR',
        etot_conv_thr = 1.0d-8,
        forc_conv_thr = 1.0d-3,
        tstress = .true.,
        tprnfor = .true.
    /
    &system
        ibrav = 8,
        celldm(1) = $CD1,
        celldm(2) = $CD2,
        celldm(3) = $CD3,
        nat = 8,
        ntyp = 1,
        ecutwfc = 200,
        ecutrho = 1600,
        occupations = 'smearing',
        smearing = 'fermi-dirac',
        degauss = 3.167d-3
    /
    &electrons
        electron_maxstep = 500,
        conv_thr = 1.0d-9,
        mixing_mode = 'TF',
        mixing_beta = 0.55,
        diagonalization = 'david',
        diag_david_ndim = 4
    /
    ATOMIC_SPECIES
        F 18.9984 F.pbe-n-kjpaw_psl.0.1.UPF
    ATOMIC_POSITIONS {crystal}
    $AP1
    $AP2
    $AP3
    $AP4
    $AP5
    $AP6
    $AP7
    $AP8
    K_POINTS {automatic}
        16 16 8 0 0 0
    FINAL
```

Manual Approximation SCF

Cmca 8 atoms - SCF Results:

```
(base) max@qmobile:~/Fluor/02-References$ grep ! 64-Cmca/SCF-* .out
64-Cmca/SCF-1.0-TPa-64.out:! total energy      = -468.99789477 Ry
64-Cmca/SCF-2.0-TPa-64.out:! total energy      = -465.40901677 Ry
64-Cmca/SCF-2.5-TPa-64.out:! total energy      = -463.78865730 Ry
64-Cmca/SCF-3.0-TPa-64.out:! total energy      = -462.24987173 Ry
64-Cmca/SCF-3.5-TPa-64.out:! total energy      = -460.77830099 Ry
64-Cmca/SCF-4.0-TPa-64.out:! total energy      = -459.36348851 Ry
64-Cmca/SCF-4.5-TPa-64.out:! total energy      = -457.99713451 Ry
64-Cmca/SCF-5.0-TPa-64.out:! total energy      = -456.67383600 Ry
```

```
(base) max@qmobile:~/Fluor/02-References$ grep "PWSCF" : 64-Cmca/SCF-* .out
64-Cmca/SCF-1.0-TPa-64.out: PWSCF : 5m35.98s CPU 6m11.20s WALL
64-Cmca/SCF-2.0-TPa-64.out: PWSCF : 4m13.70s CPU 4m37.06s WALL
64-Cmca/SCF-2.5-TPa-64.out: PWSCF : 4m 3.46s CPU 4m17.81s WALL
64-Cmca/SCF-3.0-TPa-64.out: PWSCF : 3m54.45s CPU 4m 0.38s WALL
64-Cmca/SCF-3.5-TPa-64.out: PWSCF : 3m47.23s CPU 4m12.56s WALL
64-Cmca/SCF-4.0-TPa-64.out: PWSCF : 3m41.34s CPU 4m 1.45s WALL
64-Cmca/SCF-4.5-TPa-64.out: PWSCF : 3m35.92s CPU 3m43.84s WALL
64-Cmca/SCF-5.0-TPa-64.out: PWSCF : 3m15.91s CPU 3m23.61s WALL
```



Manual Approximation Phonons

```
#!/bin/bash
#SBATCH --job-name=PH-08-64
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=80
#SBATCH --time=48:00:00
#SBATCH --partition=big_node

#Selecting module
module purge
module load QuantumExpresso/6.7.0
```

```
for P in 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.0
do
#####
# SCF Calculation
#####

...
mpirun pw.x -inp SCF-$P-TPa-64.in > SCF-$P-TPa-64.out
#####
# Phonon Calculation
#####

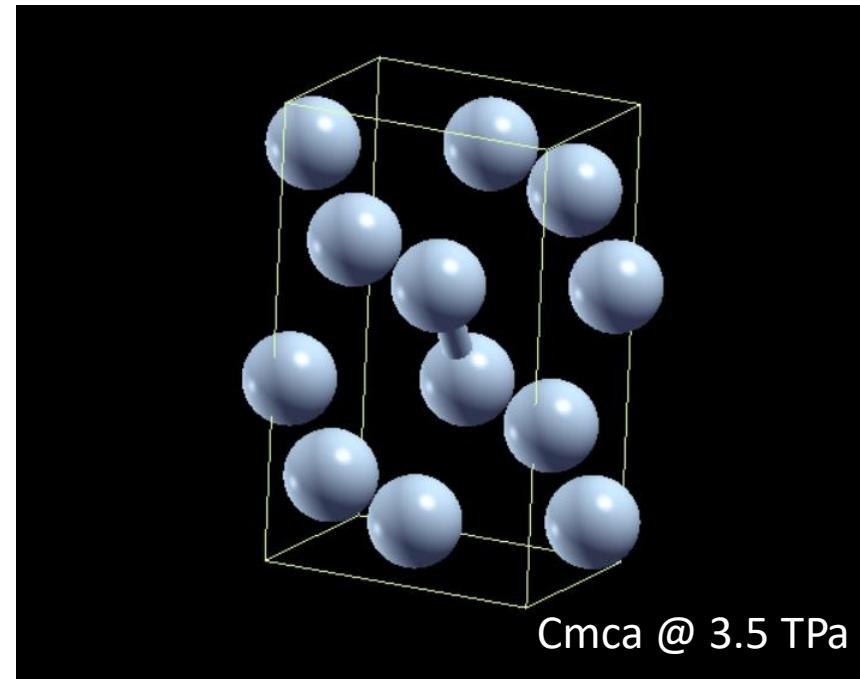
cat > PHonon-$P-TPa-64.in << FINAL
Phonons_of_64-$P-TPa
&INPUTPH
    tr2_ph = 1.0d-14 ,
    prefix = 'F8_64' ,
    max_seconds = 1.6d5 ,
    recover = .true. ,
    ldisp = .true. ,
    nq1 = 1 ,
    nq2 = 2 ,
    nq3 = 1 ,
    amass(1) = 18.9984 ,
    outdir = '$SCRATCH_DIR' ,
    fildyn = 'DynamicalMatrix-$P-TPa-64.dyn'
/
FINAL

mpirun ph.x -inp PHonon-$P-TPa-64.in > PHonon-$P-TPa-64.out
```

Manual Approximation Phonons

Cmca 8 atoms - Phonons Results:

```
Phonons-1.0-TPa-64/Phonon-1.0-TPa-64.out: PHONON : 18h 9m CPU 19h47m WALL
Phonons-1.0-TPa-64/Phonon-1.0-TPa-64.out: PHONON : 18h 9m CPU 19h47m WALL
Phonons-2.0-TPa-64/Phonon-2.0-TPa-64.out: PHONON : 13h37m CPU 15h 2m WALL
Phonons-2.0-TPa-64/Phonon-2.0-TPa-64.out: PHONON : 13h37m CPU 15h 2m WALL
Phonons-2.5-TPa-64/Phonon-2.5-TPa-64.out: PHONON : 12h21m CPU 13h45m WALL
Phonons-2.5-TPa-64/Phonon-2.5-TPa-64.out: PHONON : 12h21m CPU 13h45m WALL
Phonons-3.0-TPa-64/Phonon-3.0-TPa-64.out: PHONON : 11h52m CPU 12h41m WALL
Phonons-3.0-TPa-64/Phonon-3.0-TPa-64.out: PHONON : 11h52m CPU 12h41m WALL
Phonons-3.5-TPa-64/Phonon-3.5-TPa-64.out: PHONON : 11h10m CPU 11h57m WALL
Phonons-3.5-TPa-64/Phonon-3.5-TPa-64.out: PHONON : 11h10m CPU 11h57m WALL
Phonons-4.0-TPa-64/Phonon-4.0-TPa-64.out: PHONON : 11h 2m CPU 11h45m WALL
Phonons-4.0-TPa-64/Phonon-4.0-TPa-64.out: PHONON : 11h 2m CPU 11h45m WALL
Phonons-4.5-TPa-64/Phonon-4.5-TPa-64.out: PHONON : 10h39m CPU 11h21m WALL
Phonons-4.5-TPa-64/Phonon-4.5-TPa-64.out: PHONON : 10h39m CPU 11h21m WALL
Phonons-5.0-TPa-64/Phonon-5.0-TPa-64.out: PHONON : 9h14m CPU 10h 3m WALL
Phonons-5.0-TPa-64/Phonon-5.0-TPa-64.out: PHONON : 9h14m CPU 10h 3m WALL
```



Manual Approximation After Phonons Post-Processing

```
for P in 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.0
do

#####
# DynMat Calculation
#####

cp DynamicalMatrix-$P-TPa-64.dyn1 DynamicalMatrix-$P-TPa-64.dyn1-Original

cat > DynMat-$P-TPa-64.in << FINAL
&input
  fildyn = 'DynamicalMatrix-$P-TPa-64.dyn1',
  asr = 'crystal',
  filout = 'DynamicalMatrix-$P-TPa-64.dyn1-Corrected',
  filxsf = 'DynamicalMatrix-$P-TPa-64.dyn1-Corrected.axsf',
/
FINAL

dynmat.x -inp DynMat-$P-TPa-64.in > DynMat-$P-TPa-64.out

sed -n 1,279p DynamicalMatrix-$P-TPa-64.dyn1-Original > DynamicalMatrix-$P-TPa-64.dyn1
sed -n 5,231p DynamicalMatrix-$P-TPa-64.dyn1-Corrected >> DynamicalMatrix-$P-TPa-64.dyn1

#####
# Q2R Calculation
#####

cat > Q2R-$P-TPa-64.in << FINAL
&input
  fildyn = 'DynamicalMatrix-$P-TPa-64.dyn',
  zasr = 'simple',
  flfrc = 'ForceConstants-$P-TPa-64.fc',
/
FINAL

q2r.x < Q2R-$P-TPa-64.in > Q2R-$P-TPa-64.out
```

Manual Approximation PDOS

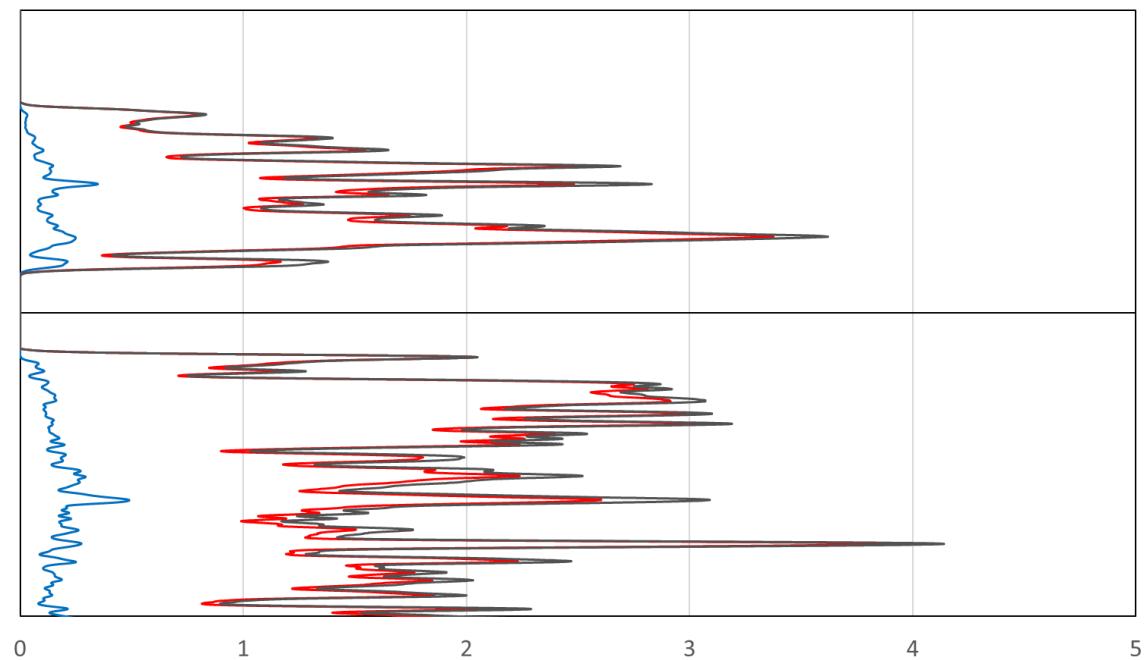
Cmca 8 atoms - PDOS Results:

```
#####
# Phonon DOS
#####

cat > PhononDOS-$P-TPa-64.in << FINAL
&input
    asr = 'crystal' ,
    dos = .true. ,
    amass(1) = 18.9984 ,
    flfrc = 'ForceConstants-$P-TPa-64.fc' ,
    fldos = 'PHDOS-$P-TPa-64.dat' ,
    nk1 = $q1 ,
    nk2 = $q2 ,
    nk3 = $q1
/
FINAL

matdyn.x -inp PhononDOS-$P-TPa-64.in > PhononDOS-$P-TPa-64.out
```

Cmca @ 3.5 TPa – PDOS



Manual Approximation Phonon Dispersion

Cmca 8 atoms – Phonon Dispersion Results:

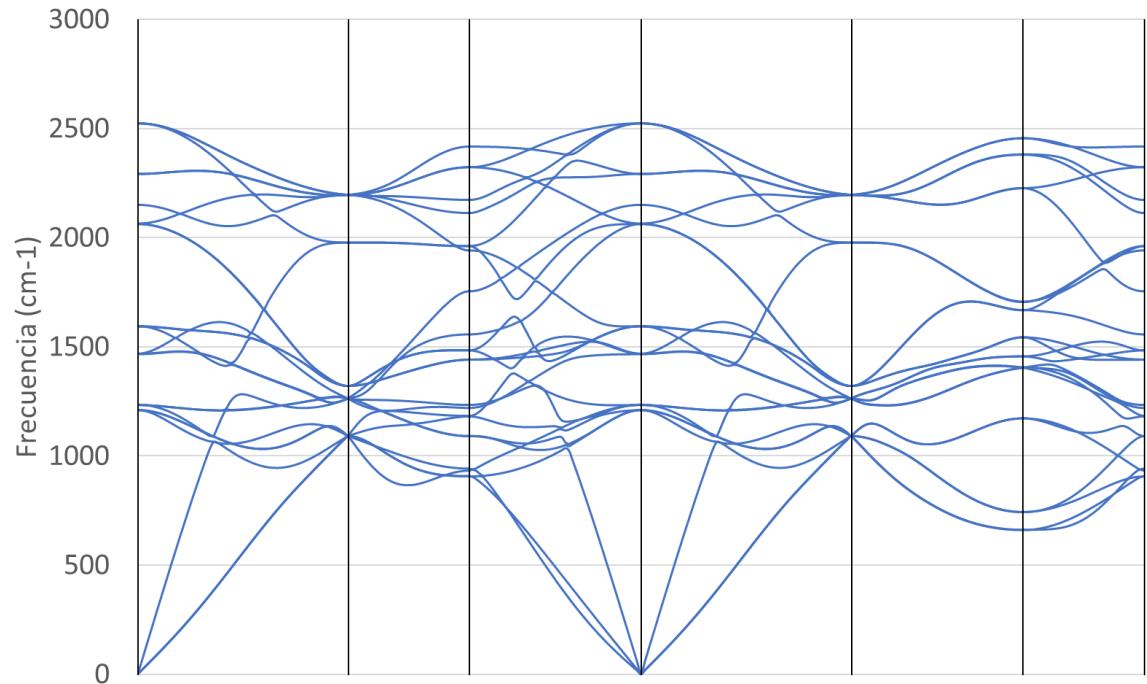
```
#####
# Phonon Bands
#####

cat > PhononBands-$P-TPa-64.in << FINAL
&input
    asr = 'crystal' ,
    amass(1) = 18.9984 ,
    dos = .false. ,
    flfrc = 'ForceConstants-$P-TPa-64.fc' ,
    flfrq = 'Frequencies-$P-TPa-64.freq' ,
    q_in_band_form = .true. ,
    q_in_cryst_coord = .true.
/
12
0.0000000000 0.0000000000 0.0000000000 50
0.5000000000 0.5000000000 0.0000000000 50
0.3743462264 0.6256537736 0.0000000000 50
0.0000000000 0.0000000000 0.0000000000 50
0.0000000000 0.0000000000 0.5000000000 50
-0.3743462264 0.3743462264 0.5000000000 50
0.5000000000 0.5000000000 0.5000000000 50
0.5000000000 0.5000000000 0.0000000000 50
0.0000000000 0.5000000000 0.0000000000 50
0.0000000000 0.5000000000 0.5000000000 50
0.0000000000 0.0000000000 0.5000000000 50
0.5000000000 0.5000000000 0.5000000000 1
FINAL

#KPoint path: Gamma - Y - F0 - Gamma - Z - B0 - T - Y - S - R - Z - T

matdyn.x -inp PhononBands-$P-TPa-64.in > PhononBands-$P-TPa-64.out
```

Cmca @ 3.5 TPa – Phonon Dispersion



Manual Approximation QHA

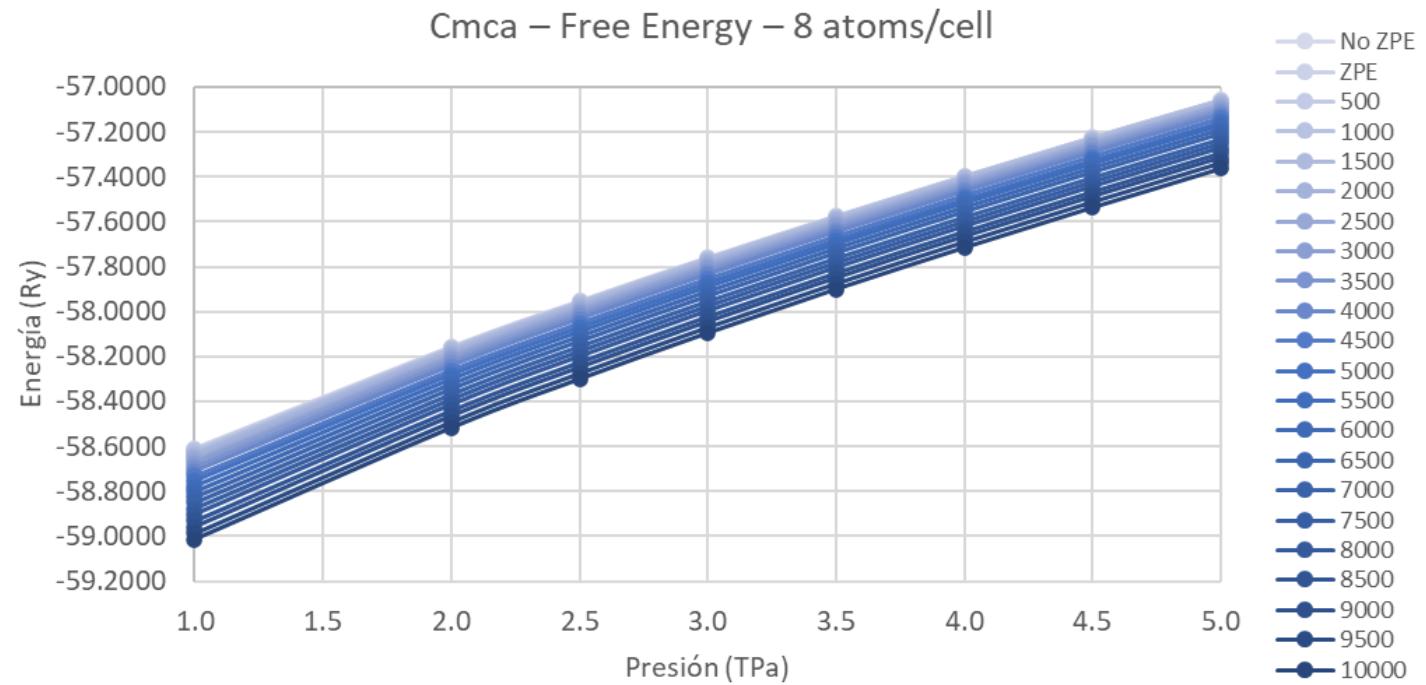
```
#####
# QHA Calculation
#####

#Removes the first line of the Phonon DOS file
sed -i '1d' PHDOS-$P-TPa-64.dat

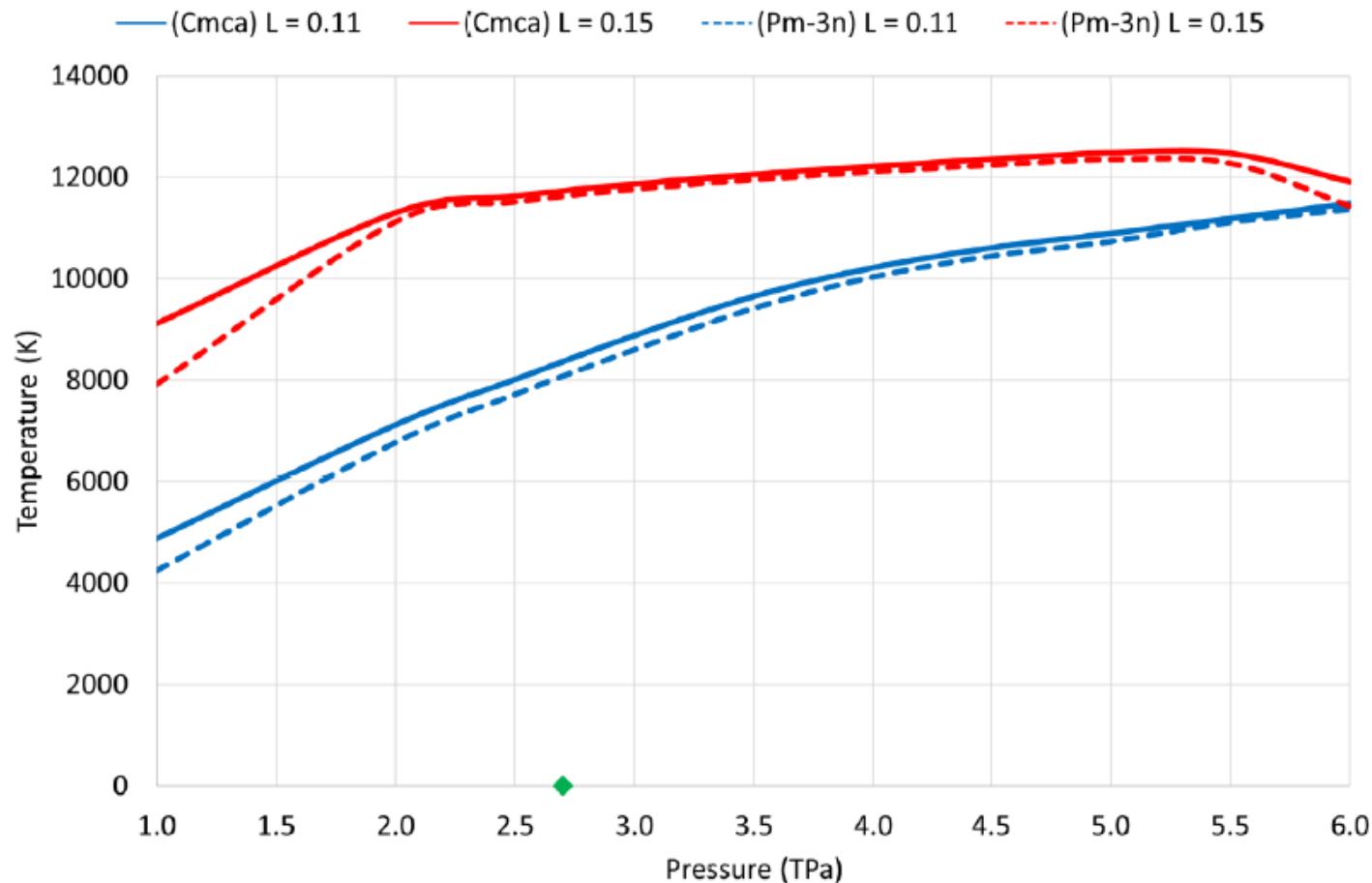
cat > QHA-$P-TPa-64.in << FINAL
PHDOS-$P-TPa-64.dat
FreeEnergy-$P-TPa-64.dat
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000
6500
7000
7500
8000
8500
9000
9500
10000
quit
FINAL

fqha.x < QHA-$P-TPa-64.in > QHA-$P-TPa-64.out
```

Cmca 8 atoms - QHA Results:



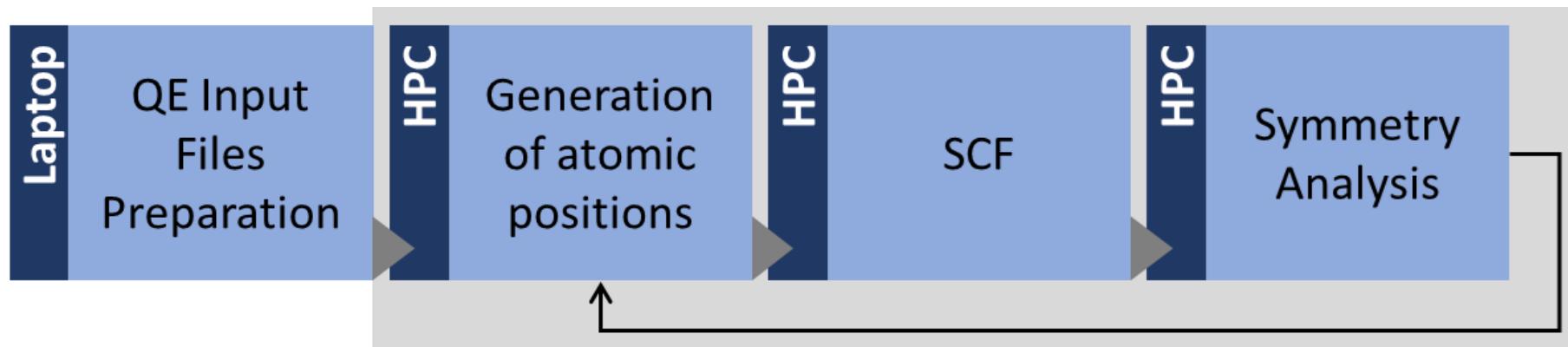
Fluorine's Melting Curve



Semi-Automatic Approximation

Structural search by means of genetic algorithms in a pressurized system

- System: Fluorine
- Specifications: 2, 4, 6, and 8 atoms/cell; Pressure: 3.5 TPa



Semi-Automatic Approximation QE Input File Preparation

```
#####
### PREPARING QE FILES FOR USPEX #####
#####

### QE - 1st Run ###

cat > qEspresso_options_1 << FINAL
&CONTROL
  calculation = 'relax',
  restart_mode = 'from_scratch',
  prefix = 'fluor',
  pseudo_dir = './',
  outdir = './',
  tstress = .true. ,
  tprnfor = .true.,
  wf_collect = .false.,
  nstep = 250 ,
  disk_io = 'none'
/
&SYSTEM
  ibrav = 0 ,
  ecutwfc = 150 ,
  ecutrho = 1500 ,
  nosym = .true. ,
  occupations = 'smearing',
  smearing = 'gaussian' ,
  degauss = 0.02
/
&ELECTRONS
  conv_thr = 5.0d-04,
  mixing_beta = 0.5,
  electron_maxstep = 250
/
&IONS
  ion_dynamics = 'bfgs',
/
```

```
#####
### PREPARING QE FILES FOR USPEX #####
#####

### QE - 2nd Run ###

cat > qEspresso_options_2 << FINAL
&CONTROL
  calculation = 'relax',
  restart_mode = 'from_scratch',
  prefix = 'fluor',
  pseudo_dir = './',
  outdir = './',
  tstress = .true. ,
  tprnfor = .true.,
  wf_collect = .false.,
  nstep = 250 ,
  disk_io = 'none'
/
&SYSTEM
  ibrav = 0 ,
  ecutwfc = 150 ,
  ecutrho = 1500 ,
  nosym = .true. ,
  occupations = 'smearing',
  smearing = 'gaussian' ,
  degauss = 0.02
/
&ELECTRONS
  conv_thr = 1.0d-06,
  mixing_beta = 0.5,
  electron_maxstep = 250
/
&IONS
  ion_dynamics = 'bfgs',
/
```

```
#####
### PREPARING QE FILES FOR USPEX #####
#####

### QE - 3rd Run ###

cat > qEspresso_options_3 << FINAL
&CONTROL
  calculation = 'relax',
  restart_mode = 'from_scratch',
  prefix = 'fluor',
  pseudo_dir = './',
  outdir = './',
  tstress = .true. ,
  tprnfor = .true.,
  wf_collect = .false.,
  nstep = 250 ,
  disk_io = 'none'
/
&SYSTEM
  ibrav = 0 ,
  ecutwfc = 150 ,
  ecutrho = 1500 ,
  nosym = .true. ,
  occupations = 'smearing',
  smearing = 'gaussian' ,
  degauss = 0.02
/
&ELECTRONS
  conv_thr = 1.0d-08,
  mixing_beta = 0.5,
  electron_maxstep = 250
/
&IONS
  ion_dynamics = 'bfgs',
/
```

```
#####
### PREPARING QE FILES FOR USPEX #####
#####

### QE - 4th Run ###

cat > qEspresso_options_4 << FINAL
&CONTROL
  calculation = 'relax',
  restart_mode = 'from_scratch',
  prefix = 'fluor',
  pseudo_dir = './',
  outdir = './',
  tstress = .true. ,
  tprnfor = .true.,
  wf_collect = .false.,
  nstep = 250 ,
  disk_io = 'none'
/
&SYSTEM
  ibrav = 0 ,
  ecutwfc = 150 ,
  ecutrho = 1500 ,
  nosym = .true. ,
  occupations = 'smearing',
  smearing = 'gaussian' ,
  degauss = 0.02
/
&ELECTRONS
  conv_thr = 1.0d-10,
  mixing_beta = 0.5,
  electron_maxstep = 250
/
&IONS
  ion_dynamics = 'bfgs',
/
```

Semi-Automatic Approximation USPEX

```
#!/bin/bash
#SBATCH --job-name=U-3.5T-8a
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=20
#SBATCH --time=144:00:00
#SBATCH --partition=normal

#Selecting module
module purge
module load QuantumExpresso/6.7.0
```

```
#####
### PREPARING USPEX INPUT FILE #####
#####

cat > INPUT.txt << FINAL
*****
*   TYPE OF RUN AND SYSTEM           *
*****
USPEX  : calculationMethod (USPEX, VCNEB, META)
300   : calculationType (dimension: 0-3; molecule: 0/1; varcomp: 0/1)
1     : AutoFrac

% optType
1
% EndOptType

% atomType
F
% EndAtomType

% numSpecies
$NAT
% EndNumSpecies

% symmetries
2-230
% endSymmetries
*****
*          POPULATION            *
*****
30   : populationSize
30   : initialPopSize
50   : numGenerations
15   : stopCrit
0    : reoptOld
0.6  : bestFrac
*****
```

```
*****
*          VARIATION OPERATORS      *
*****
0.50  : fracGene
0.30  : fracAtomsMut
0.20  : fracRand
0.00  : fracPerm
0.00  : fracLatMut
*****
*          DETAILS OF AB INITIO CALCULATIONS  *
*****
% abinitioCode
8 8 8 8
% ENDabinit

% KresolStart
0.20 0.16 0.12 0.08
% Kresolend

% commandExecutable
mpirun pw.x < qe.in > output
% EndExecutable

$P   : ExternalPressure
1     : numParallelCalcs
0     : whichCluster

FINAL

#####
USPEX -r
```

Semi-Automatic Approximation USPEX

Structural Search at 3.5 TPa Results:

```
(base) max@qmobile:~/Fluor/01-USPEX/P-3.5-TPa$ grep "Job Starts at" ??-atoms/results1/OUTPUT.txt
02-atoms/results1/OUTPUT.txt:          Job Starts at      03-Feb-2022 12:52:34
04-atoms/results1/OUTPUT.txt:          Job Starts at      12-Feb-2022 11:07:50
06-atoms/results1/OUTPUT.txt:          Job Starts at      03-Mar-2022 08:53:32
08-atoms/results1/OUTPUT.txt:          Job Starts at      10-Mar-2022 11:07:24
```

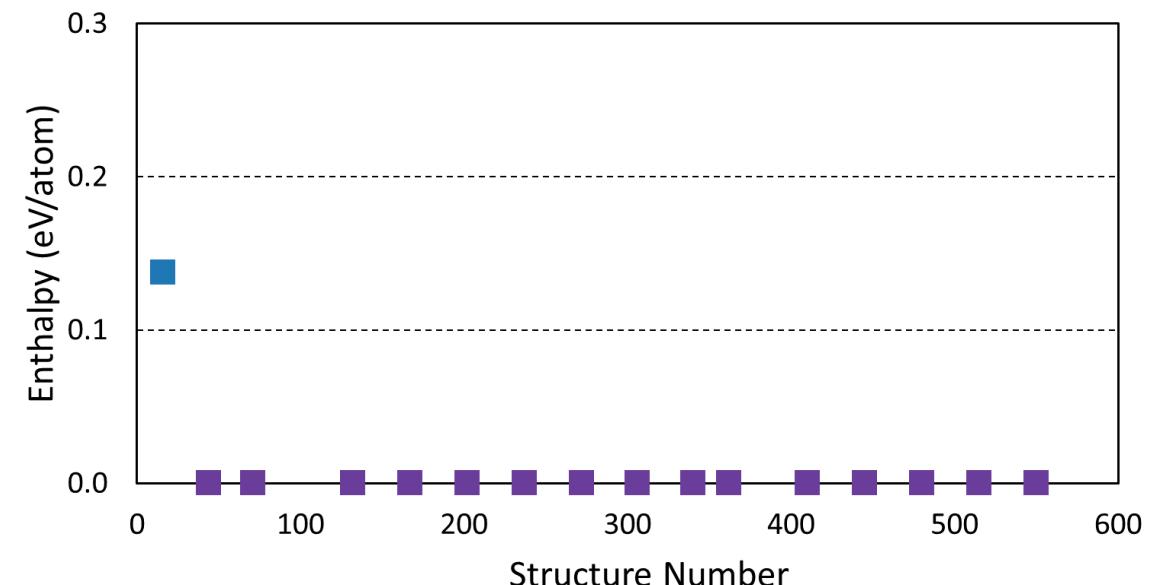
```
(base) max@qmobile:~/Fluor/01-USPEX/P-3.5-TPa$ grep "Job Finished at" ??-atoms/results1/OUTPUT.txt
02-atoms/results1/OUTPUT.txt:          Job Finished at    03-Feb-2022 22:40:29
04-atoms/results1/OUTPUT.txt:          Job Finished at    13-Feb-2022 17:48:00
06-atoms/results1/OUTPUT.txt:          Job Finished at    06-Mar-2022 22:00:47
08-atoms/results1/OUTPUT.txt:          Job Finished at    13-Mar-2022 21:29:50
```

USPEX CALCULATIONS

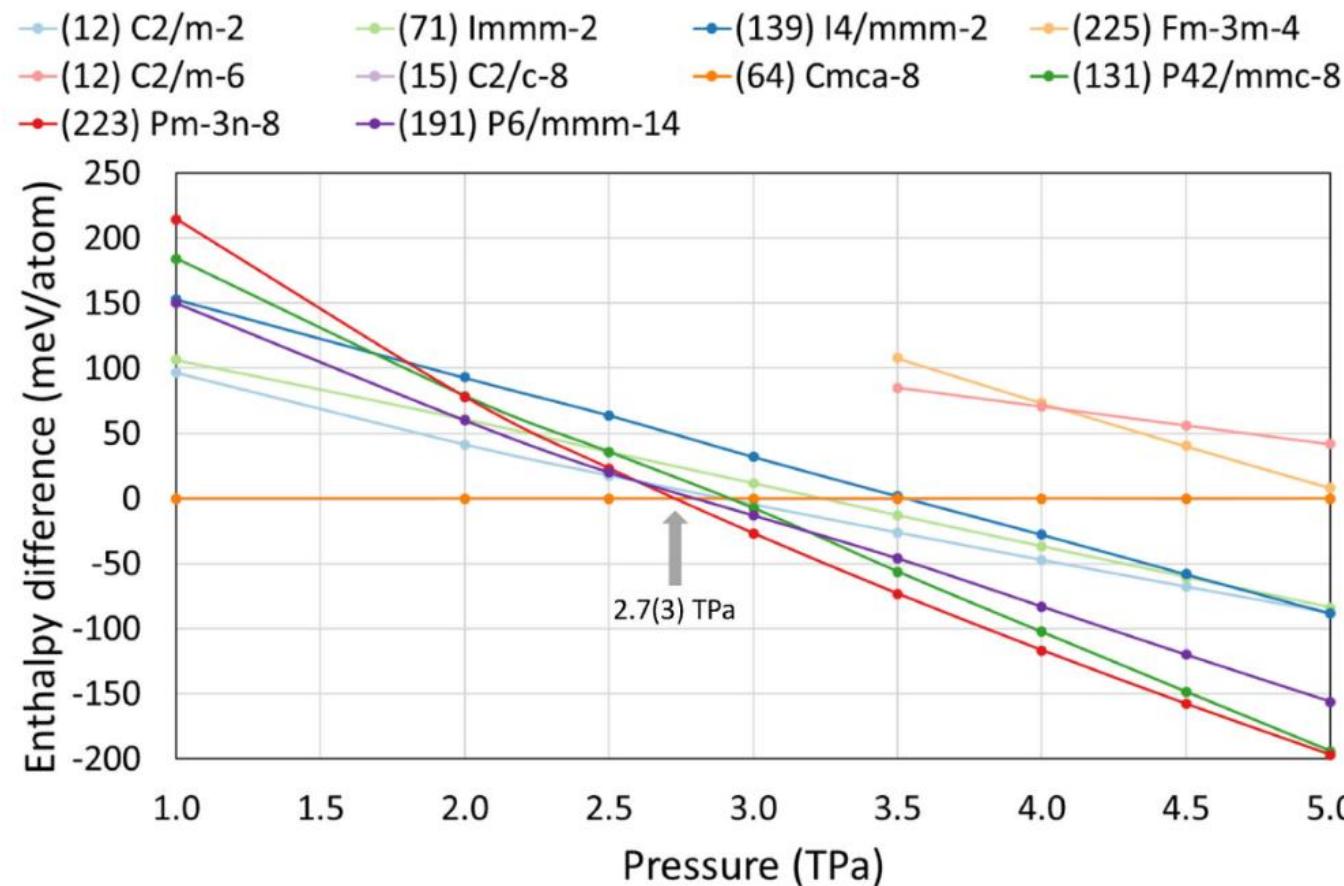
P [Tpa]	atoms /cell			
	2	4	6	8
3.5	3-feb-22 9h 48min	13-feb-22 1d 6h 41min	6-mar-22 3d 13h 7min	13-mar-22 3d 10h 22min

Structure Prediction - 3.5 TPa

■ (139) I4/mmm ■ (223) Pm-3n



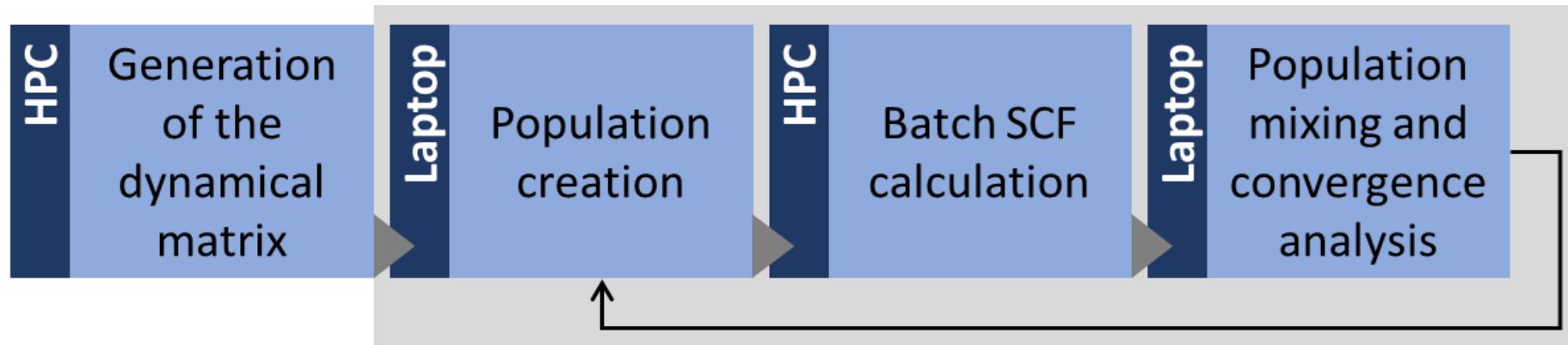
Semi-Automatic Approximation USPEX



Automatic Approximation

Anharmonic vibrational properties at finite temperature in a pressurized system

- System: Diamond (carbon)
- Specifications: 2 atoms/cell; Pressure: 2 TPa; Temperatures: 0K, 500K, 2000K, 3000K, 4000K...



Automatic Approximation Diamond with SSCHA

Analyzing convergence prior to automatizing

As for the Manual Approximation, also here the electronic kinetic energy (Ecut) and the reciprocal space grid (k-points) was converged. The takeaway message is that with respect to the best converged system that we tested (Ecut=200Ry, k-points=12x12x12, q-points=8x8x8) the one that we finally used provided a very similar accuracy at a fraction of its computational cost (Ecut=80Ry, k-points=8x8x8, q-points=4x4x4)

- Let's compare times for the two electronic energy calculations:

8x8x8_k-point_80Ry/Diamond.scf.out: **6.78s CPU 7.43s WALL**

12x12x12_k-point_200Ry/Diamond.scf.out: **24.73s CPU 27.69s WALL**

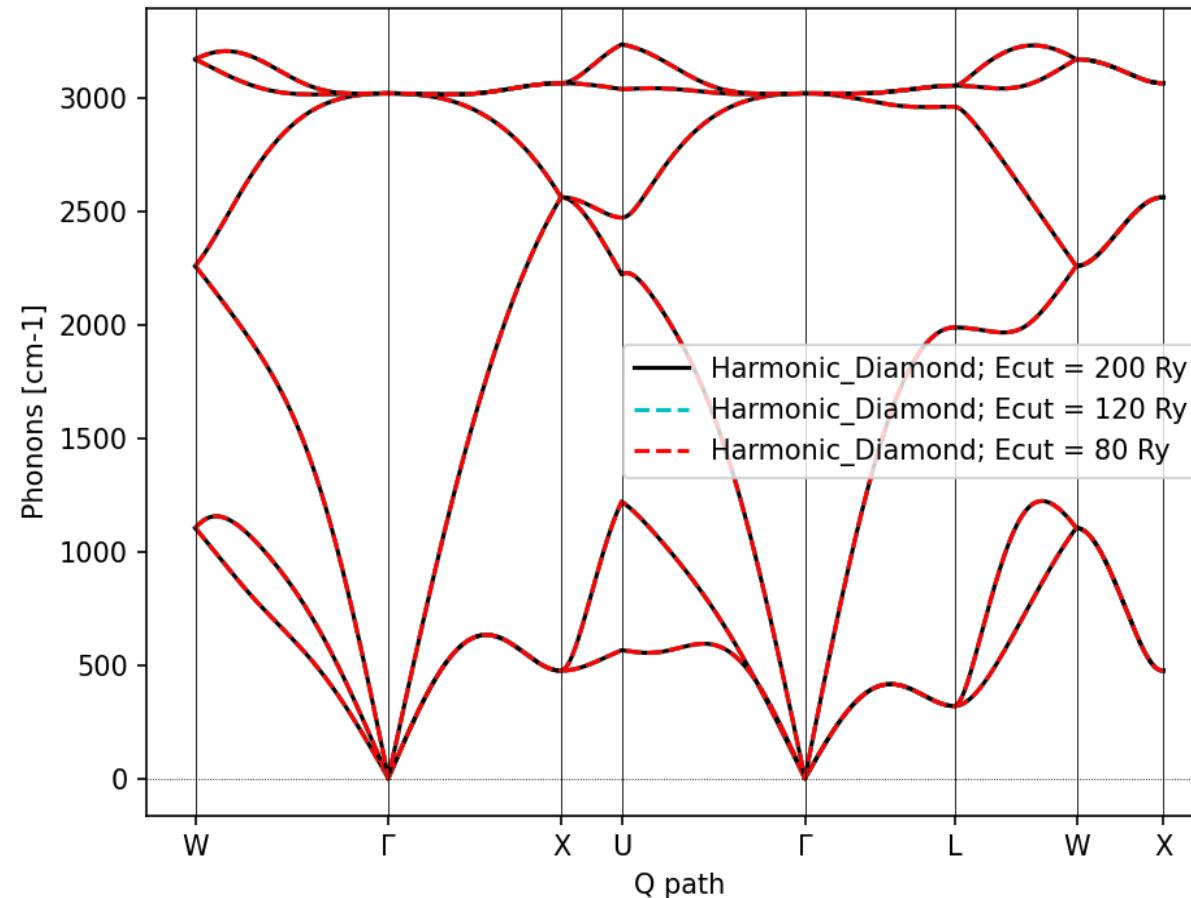
- And now the phonon frequencies:

4x4x4_q-point_80Ry/Diamond.scf.out: **13m51.22s CPU 15m39.03s WALL**

8x8x8_q-point_200Ry/Diamond.scf.out: **10h 4m CPU 11h 5m WALL**

Outcome: System's dynamical matrix

Automatic Approximation Diamond with SSCHA



Automatic Approximation Diamond with SSCHA

The screenshot shows a Jupyter Notebook interface with the title "jupyter Argo-jmtonoya_Diamond-Minimalist Last Checkpoint: 13 minutes ago (autosaved)". The notebook has tabs for File, Edit, View, Insert, Cell, Kernel, and Help. A toolbar below the tabs includes icons for file operations like Open, Save, Run, and Cell. To the right of the toolbar are buttons for Trusted and Python 3 (ipykernel). The main area contains a code cell with the following Python code:

```
In [ ]: # Initialize the DFT (Quantum Espresso) calculator for gold
# The input data is a dictionary that encodes the pw.x input file namelist
input_data = {
    'control' : {
        # Avoid writing wavefunctions on the disk
        'disk_io'      : 'None',
        # Where to find the pseudopotential in the cluster
        'pseudo_dir'   : '/home/jmtonoya/pseudo',
        'outdir'       : '/home/jmtonoya/Diamond/SSCHA',
        'etot_conv_thr' : 1e-10,
        'tstress'       : True,
        'tprnfor'       : True
    },
    'system' : {
        # Specify the basis set cutoffs
        'ecutwfc'      : 80, # Cutoff for wavefunction
        'ecutrho'       : 640 # Cutoff for the density
    },
    'electrons' : {
        'conv_thr'      : 1e-9,
        'mixing_mode'   : 'TF',
        'mixing_beta'   : 0.55,
        'diagonalization': 'david',
        'diago_david_ndim': 4
    }
}

# the pseudopotential for each chemical element
# In this case just Gold
pseudopotentials = {'C' : 'C.pbe-n-kjpaw_psl.0.1.UPF'}


# the kpoints mesh for a 4x4x4 supercell that corresponds to an 8x8x8 k-grid in the primitive, and the offset
kpts = (2,2,2)
koffset = (1,1,1)
```

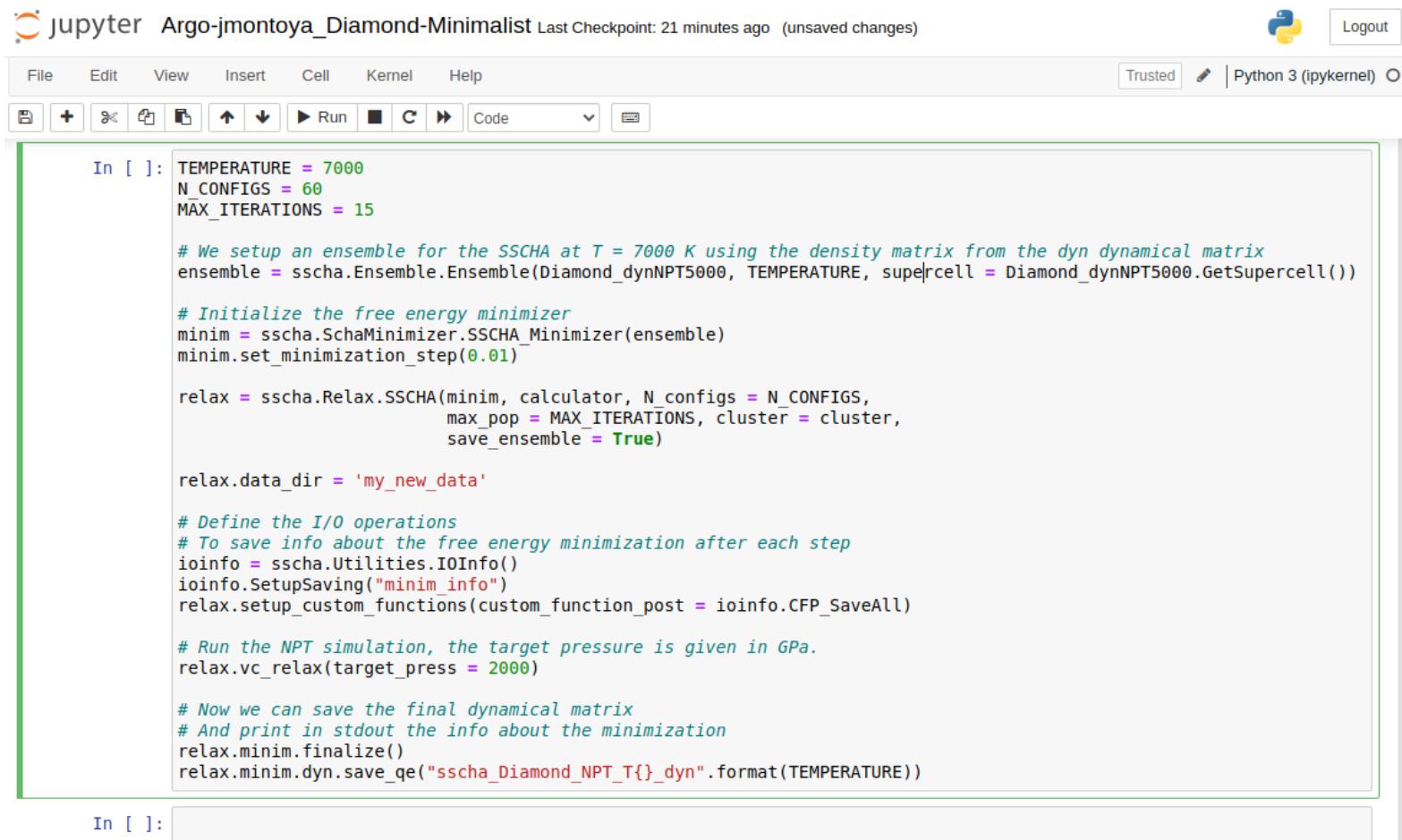
Automatic Approximation Diamond with SSCHA

The screenshot shows a Jupyter Notebook interface with the title "jupyter Argo-jmontoya_Diamond-Minimalist" and a status bar indicating "Last Checkpoint: 15 minutes ago (autosaved)". The notebook has tabs for "File", "Edit", "View", "Insert", "Cell", "Kernel", and "Help". A toolbar below the tabs includes icons for file operations like Open, Save, and Run, along with a "Code" dropdown menu. The main area displays a code cell (In []):

```
# Configure remote cluster
cluster = sscha.Cluster(hostname = 'jmontoya@argo.ictp.it', pwd = None, mpi_cmd= 'mpirun -np 40')
cluster.workdir = '/home/jmontoya/Diamond/SSCHA'
cluster.n_nodes = 1
cluster.time = '24:00:00'
cluster.n_cpu = 40
cluster.n_pool = 2
cluster.account_name = 'cmsp'
cluster.partition_name = 'cmsp'
cluster.custom_params["--ntasks-per-node"] = '40'
cluster.custom_params["--cpus-per-task"] = '1'
cluster.custom_params["--job-name"] = 'ESP'
cluster.custom_params["--err"] = 'Job_ESP.err'
cluster.custom_params["--out"] = 'Job_ESP.out'
cluster.batch_size = 1
cluster.job_number = 60
#cluster.use_partition = False
cluster.use_qos = False
#cluster.set_timeout(30)
cluster.load_modules = """
module purge
module load intel/2018
module load openmpi/4.0.0/intel
module load gnu-openmpi/fftw/3.3.4
module load espresso/6.8
export OMP_NUM_THREADS=1
export MKL_NUM_THREADS=$OMP_NUM_THREADS
export I_MPI_PIN_DOMAIN=omp
ulimit -s unlimited
"""
cluster.binary = 'pw.x -npool NPOOL -i PREFIX.pwi > PREFIX.pwo'

# Prepare the quantum espresso calculator
calculator = CC.calculators.Espresso(input_data,
                                      pseudopotentials,
                                      kpts = kpts,
                                      koffset = koffset)
```

Automatic Approximation Diamond with SSCHA



The screenshot shows a Jupyter Notebook interface with the following details:

- Title Bar:** jupyter Argo-jmowntoya_Diamond-Minimalist Last Checkpoint: 21 minutes ago (unsaved changes) Logout
- Toolbar:** File, Edit, View, Insert, Cell, Kernel, Help, Trusted, Python 3 (ipykernel)
- Code Cell:** In []:

```
TEMPERATURE = 7000
N_CONFIGS = 60
MAX_ITERATIONS = 15

# We setup an ensemble for the SSCHA at T = 7000 K using the density matrix from the dyn dynamical matrix
ensemble = sscha.Ensemble(Diamond_dynNPT5000, TEMPERATURE, supercell = Diamond_dynNPT5000.GetSupercell())

# Initialize the free energy minimizer
minim = sscha.SchaMinimizer.SSCHA_Minimizer(ensemble)
minim.set_minimization_step(0.01)

relax = sscha.Relax.SSCHA(minim, calculator, N_configs = N_CONFIGS,
                           max_pop = MAX_ITERATIONS, cluster = cluster,
                           save_ensemble = True)

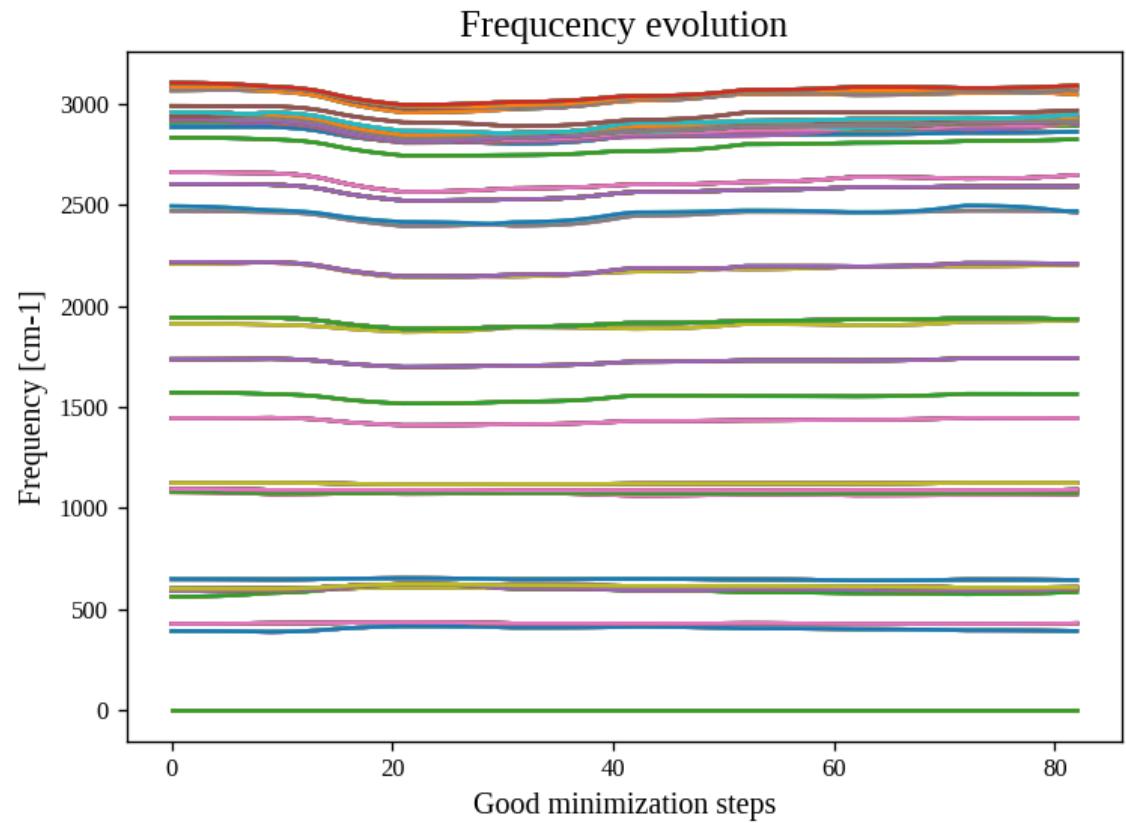
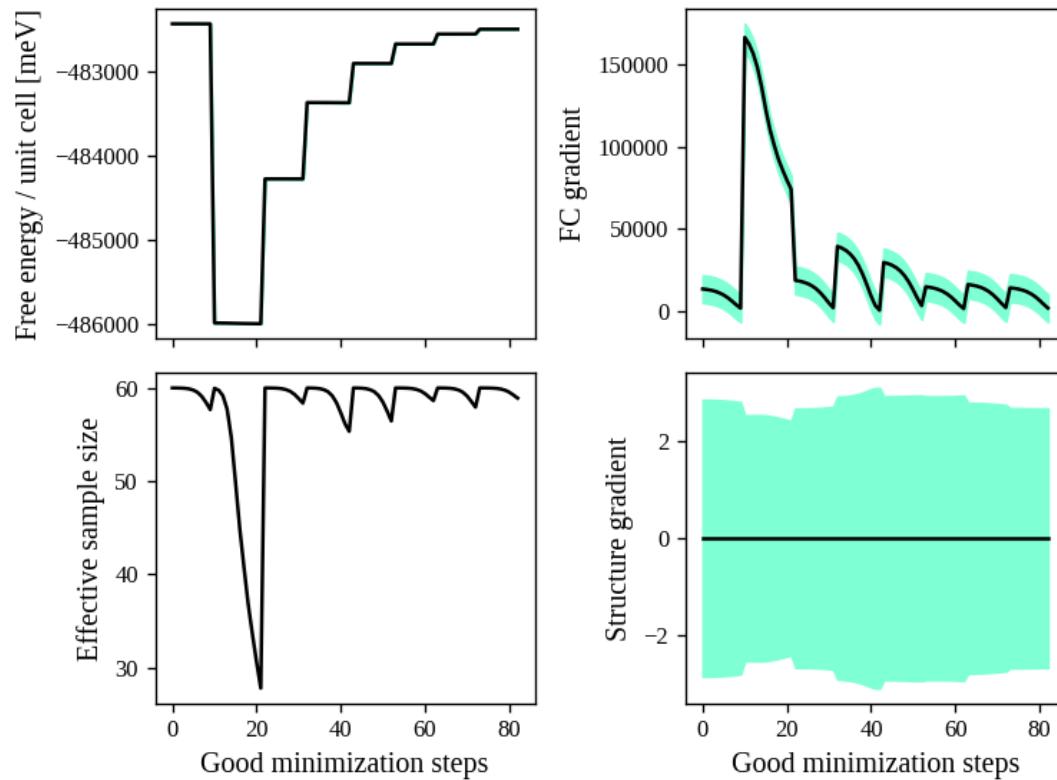
relax.data_dir = 'my_new_data'

# Define the I/O operations
# To save info about the free energy minimization after each step
ioinfo = sscha.Utilities.IOInfo()
ioinfo.SetupSaving("minim_info")
relax.setup_custom_functions(custom_function_post = ioinfo.CFP_SaveAll)

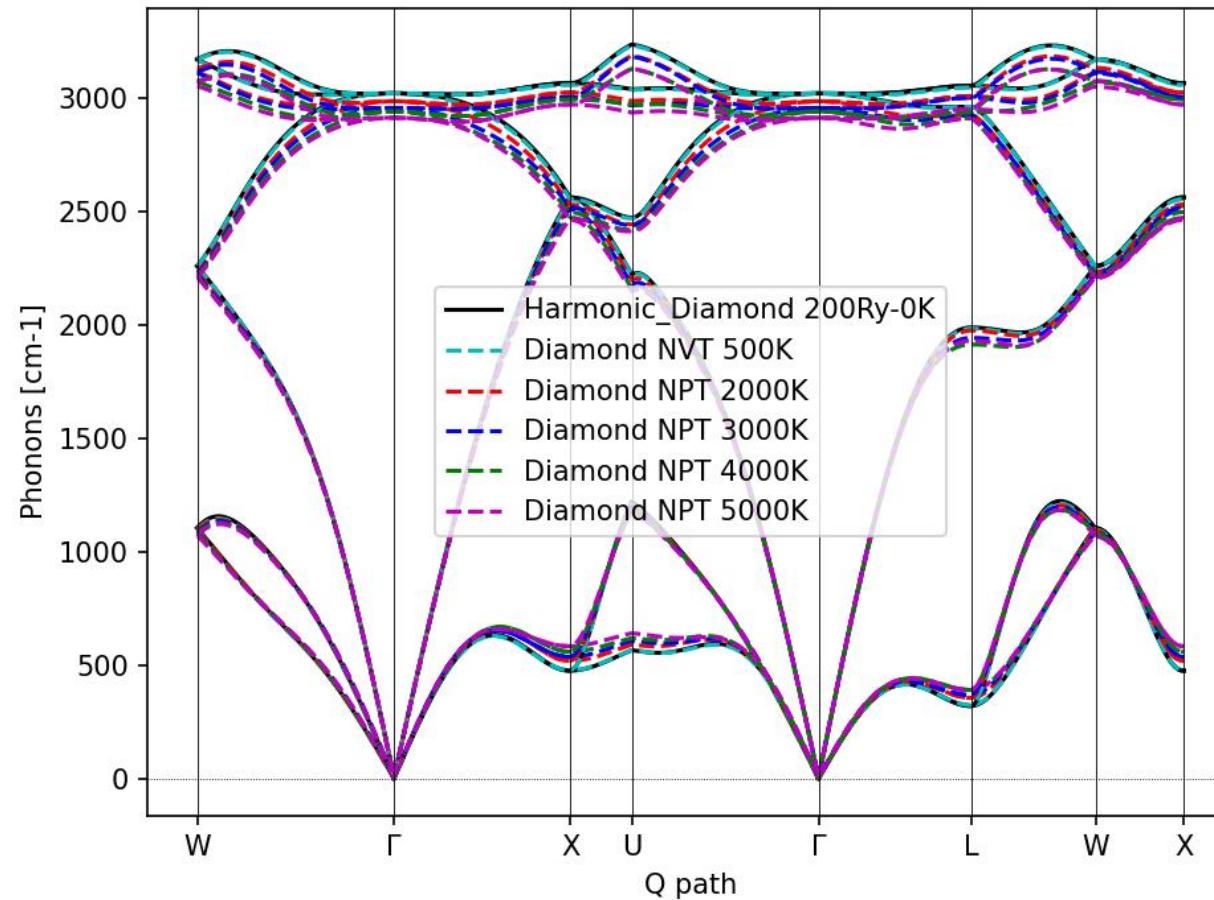
# Run the NPT simulation, the target pressure is given in GPa.
relax.vc_relax(target_press = 2000)

# Now we can save the final dynamical matrix
# And print in stdout the info about the minimization
relax.minim.finalize()
relax.minim.dyn.save_qe("sscha_Diamond_NPT_T{}_dyn".format(TEMPERATURE))
```
- Bottom Cell:** In []:

Automatic Approximation Diamond with SSCHA



Automatic Approximation Diamond with SSCHA



Summary

Summary

- Know your problem
- Know your code
- Perform tests
- Select the right hardware
- Select the best workflow
- Do "relevant" HPC stuff :-)

Acknowledgements

Acknowledgements



The Abdus Salam
**International Centre
for Theoretical Physics**

Sandro Scandolo

Associates Program



**Universidad
de Cartagena**
Fundada en 1827

HPC Facility

ROSMME Computational Resource



**MINISTERIO DE CIENCIA,
TECNOLOGÍA E INNOVACIÓN**

Convocatoria No. 891 de 2020

THANK YOU
