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Semimetallic and metallic states of crystalline molecular hydrogen

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Outline

1. Calculation method.

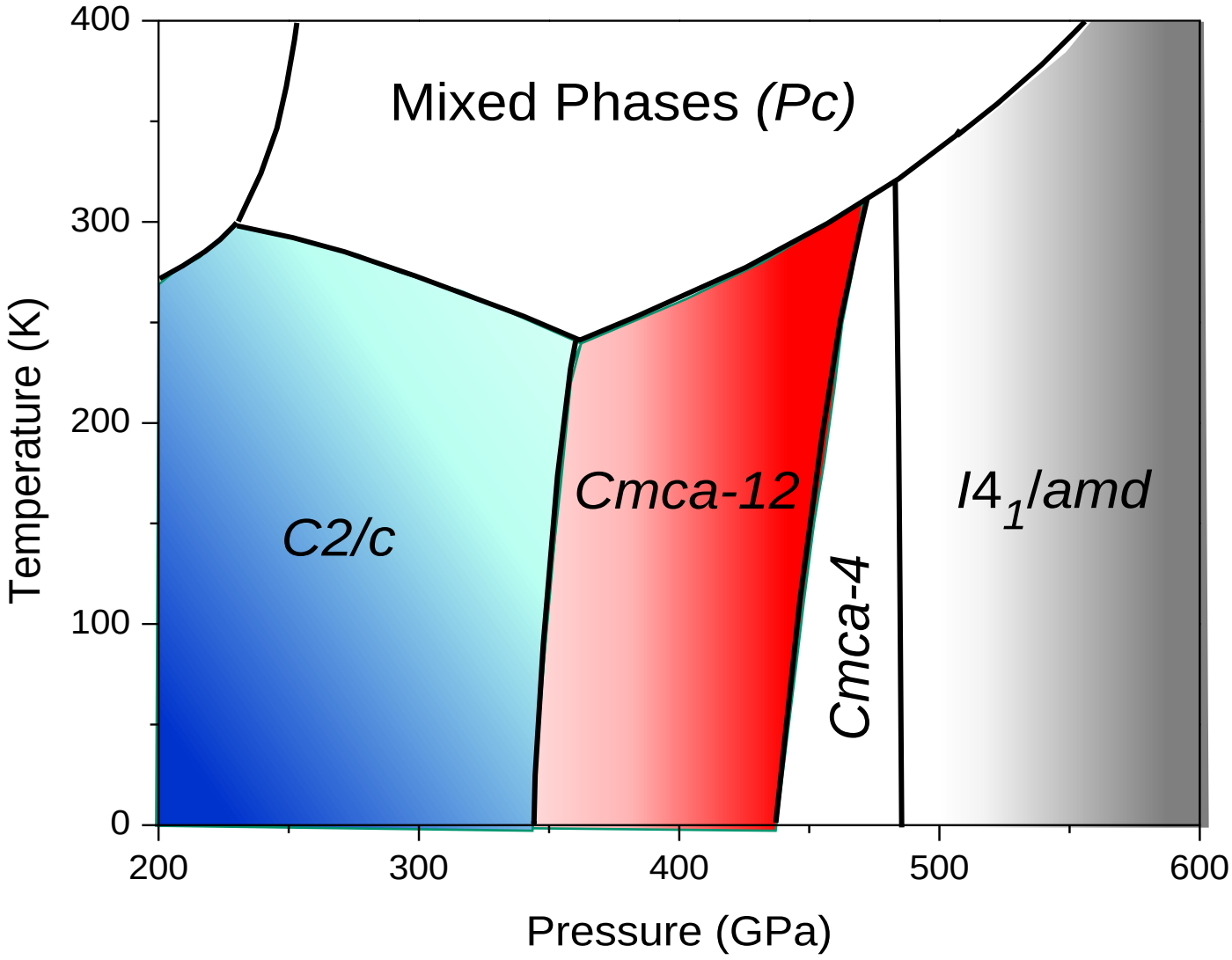
2. Molecular phase at high pressure.

3. Semimetallic states
of molecular crystalline hydrogen

4. Metallic states
of molecular crystalline hydrogen

5. Conclusions.

Theoretical phase diagram of solid hydrogen



S. Azadi et al // PRL 112, 165501 (2014)

1. Calculation method.

METHOD

1. Calculation of the ion's trajectories
determined by the solution of
the Newton's equations of motion
with forces obtained within the DFT

2. Equilibration of the system

3. Calculation of parameters of the system:
Proton-proton pair correlation function g(r)
Pressure
Conductivity, Band structure & DOS

Ab initio molecular dynamics

Classical diagnostics for ions

Correlation and auto-correlation functions

Pressure and other thermodynamic properties

Diffusion, Viscosity etc.

Ionic Conductivity

Averaging over ionic configurations

Coordinates and ionic velocities

$\mathbf{R}_I(t), \mathbf{V}_I(t)$

$\mathbf{R}_I$
$\mathbf{V}_I$

$\mathbf{V}_I(t+\Delta t)$
$\mathbf{R}_I(t+\Delta t)$

$\mathbf{F}_I$

ТФП

Wave functions,
Energy levels,
Electron density

$\psi_i \quad \varepsilon_i \quad n(\mathbf{r})$

ψ_i

ε_i

Forces $\mathbf{F}_I =$

$$-\nabla_I \left\{ E^{KS}\left[n(\mathbf{r}), \mathbf{R}_I \right] \right\} =$$

$$= -\left\langle \Psi \left| \frac{\partial H^{KS}}{\partial \mathbf{R}_I} \right| \Psi \right\rangle$$

Equations of motion

$$M_I \ddot{\mathbf{R}}_I = \mathbf{F}_I$$

Quantum diagnostics for electrons

Charge density distribution

Electric Conductivity

Reflectivity

Density of electron states

Band structure

Averaging over ionic configurations

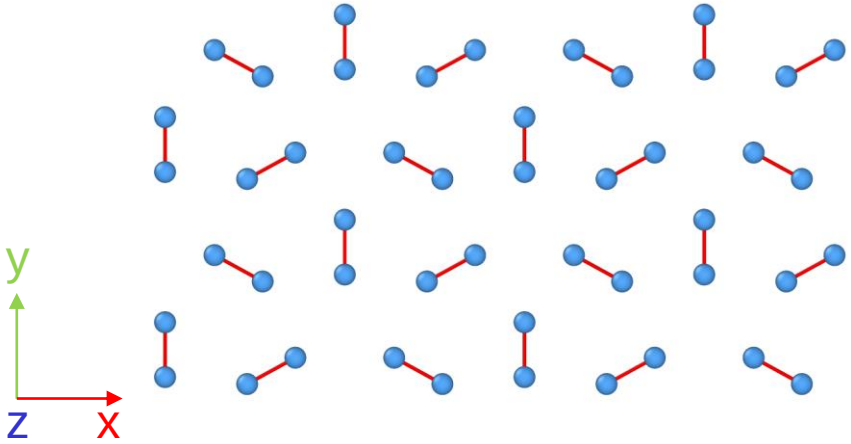
2. Molecular phase at high pressure.

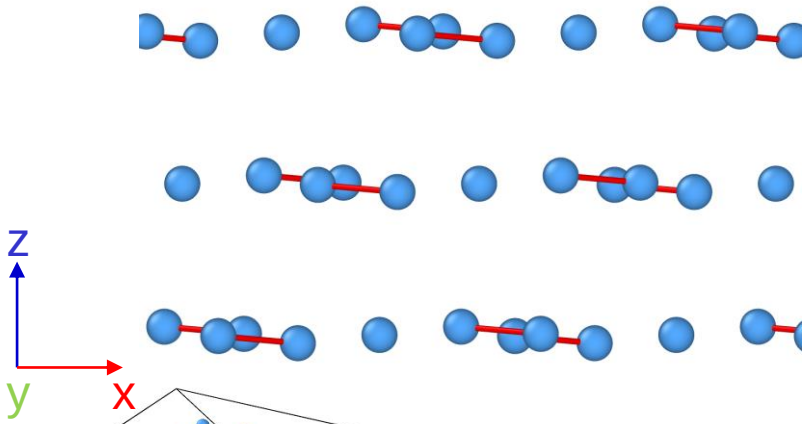
Initial configuration

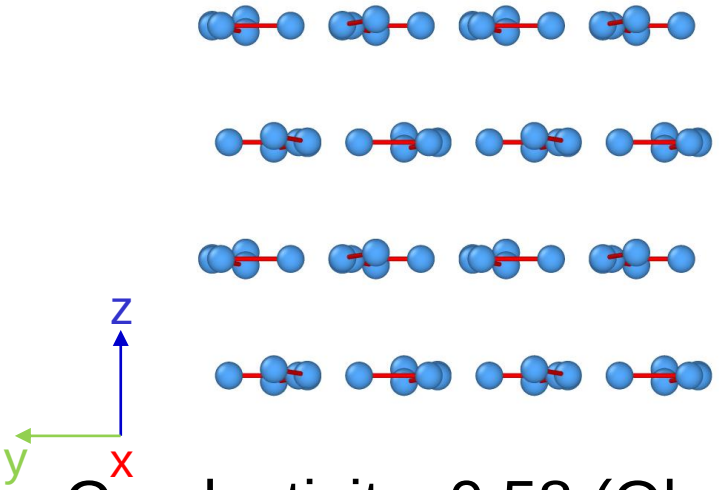
Monocline structure
with **C2/c** space group
12 atoms in the unit cell

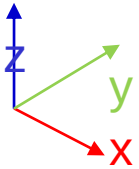
Density: 1.14 g/cm^3
Pressure: 302 GPa
Number of particles: 192

C.J. Pickard, R.J. Needs // Nature Phys. **3,** 473 (2007)





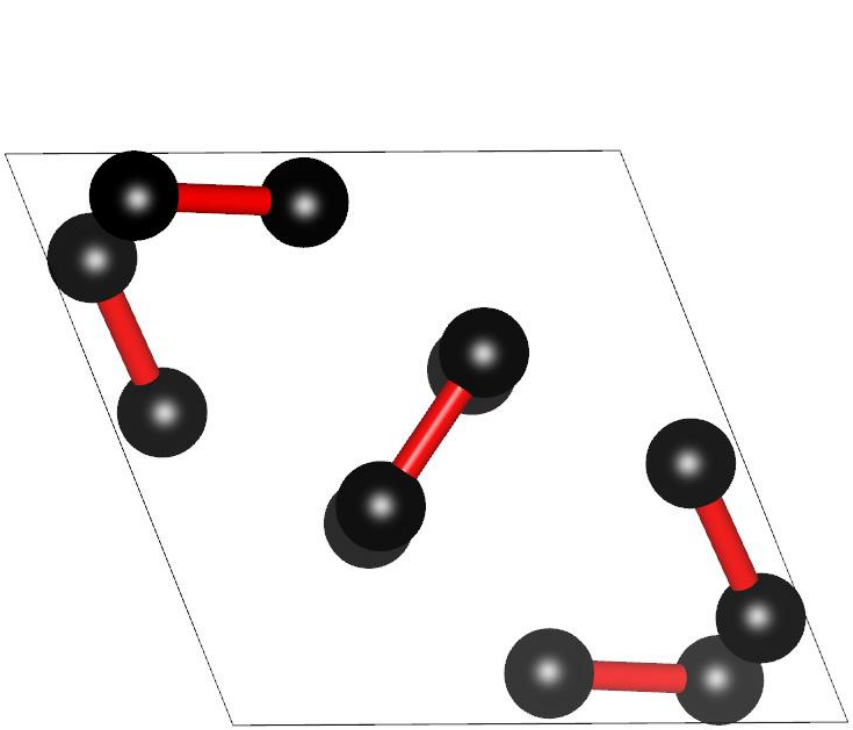




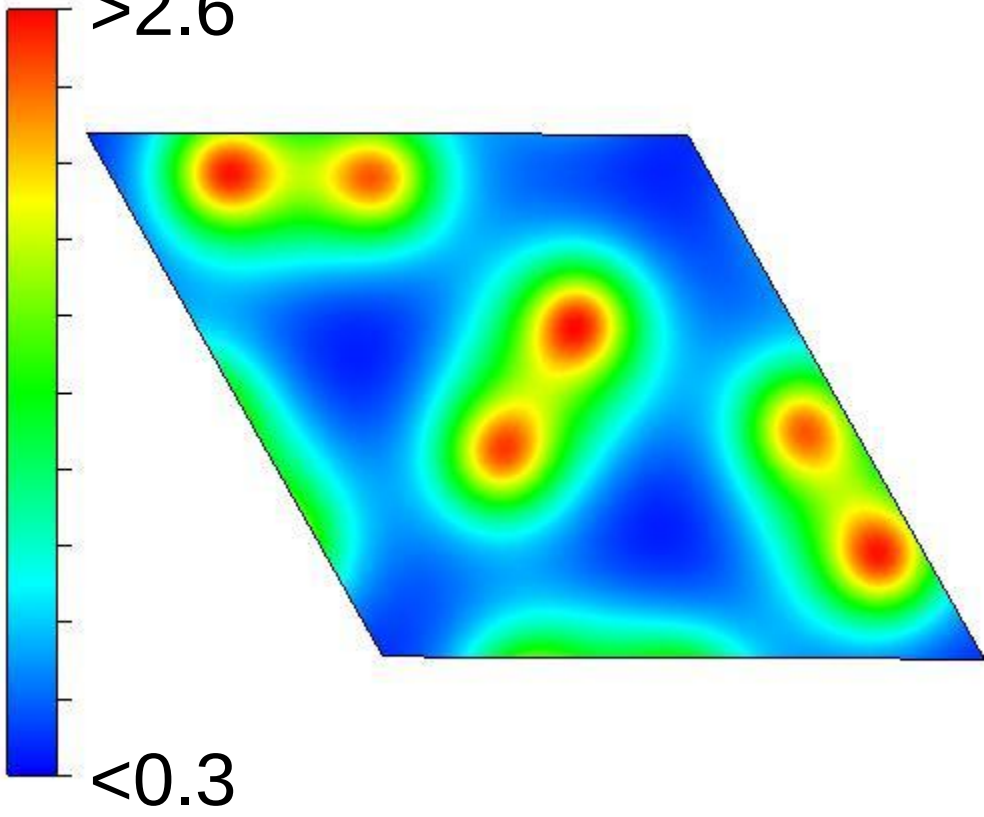
Conductivity: 0.58 (Ohm·cm)$^{-1}$

Primitive cell and charge density at pressure 302 GPa

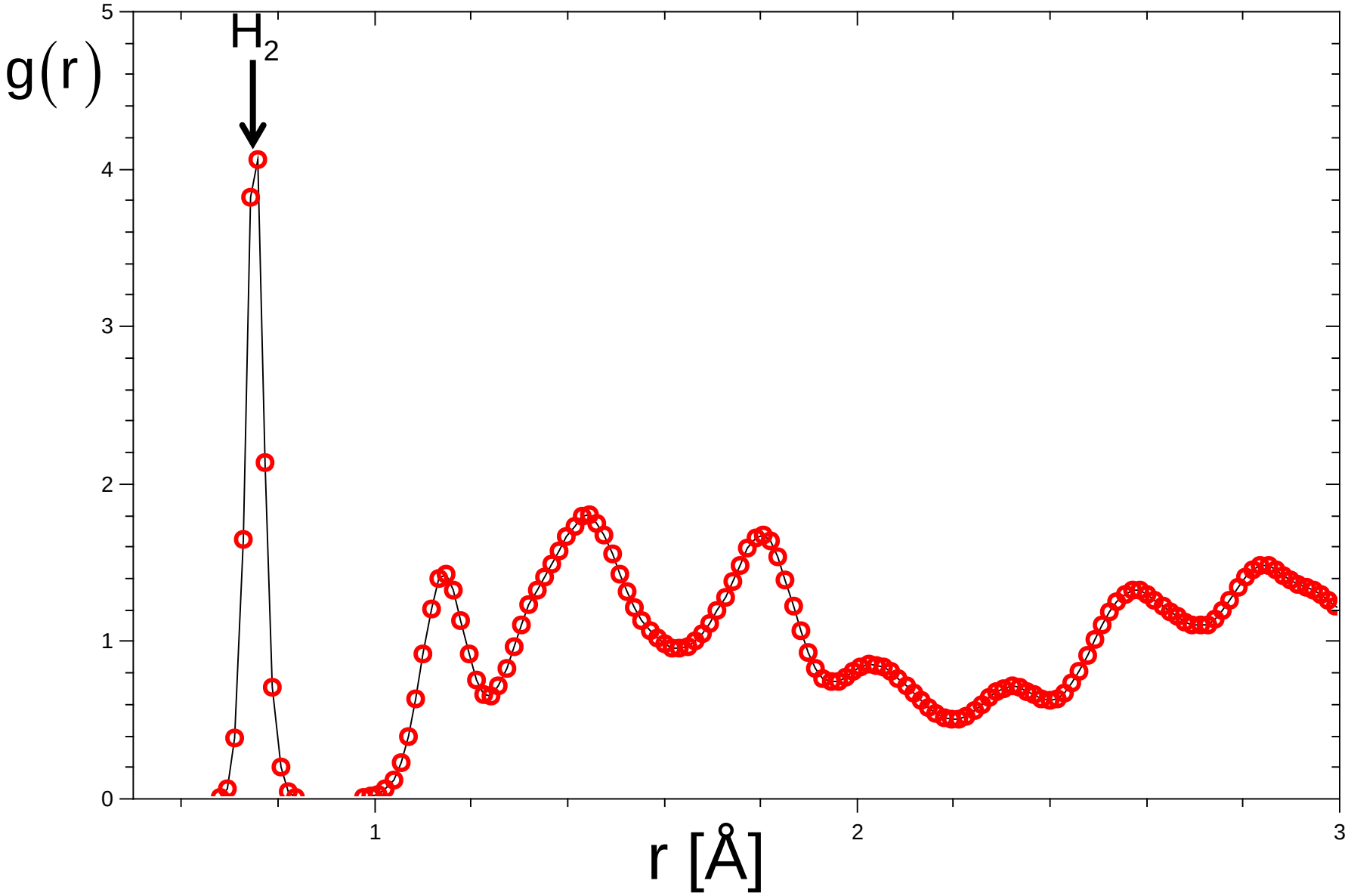
Space group: C2/c-12

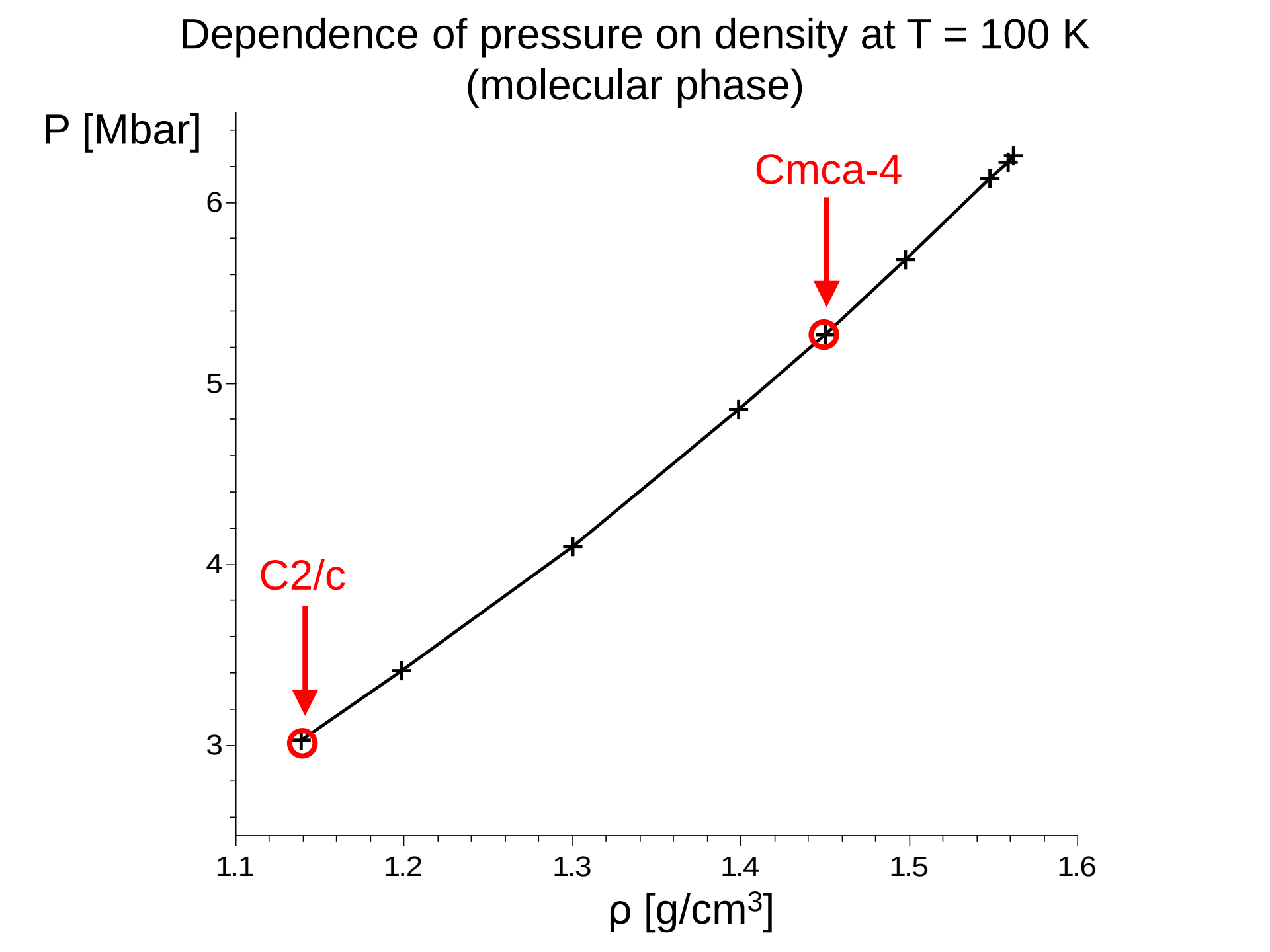


Charge density, (1/Å^3)

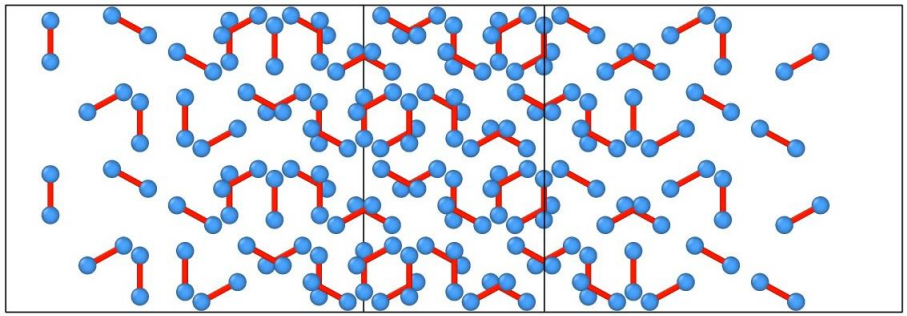


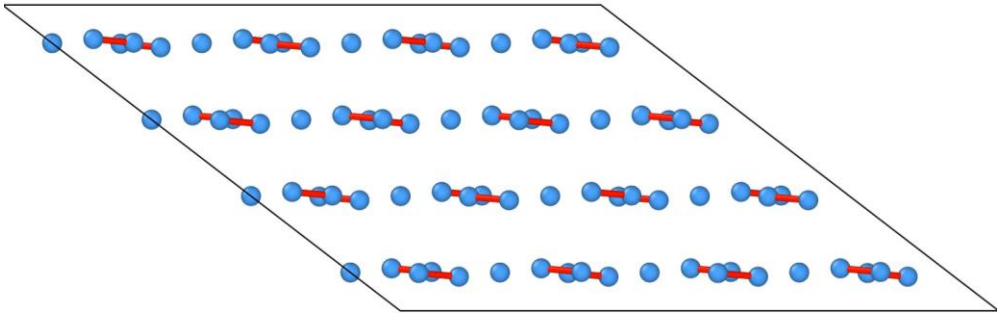
Pair correlation function at pressure 302 GPa

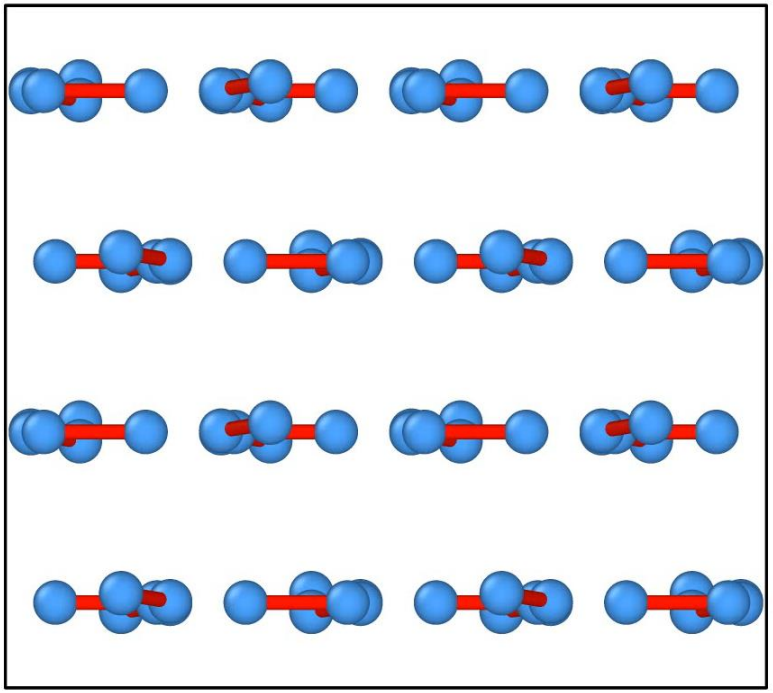


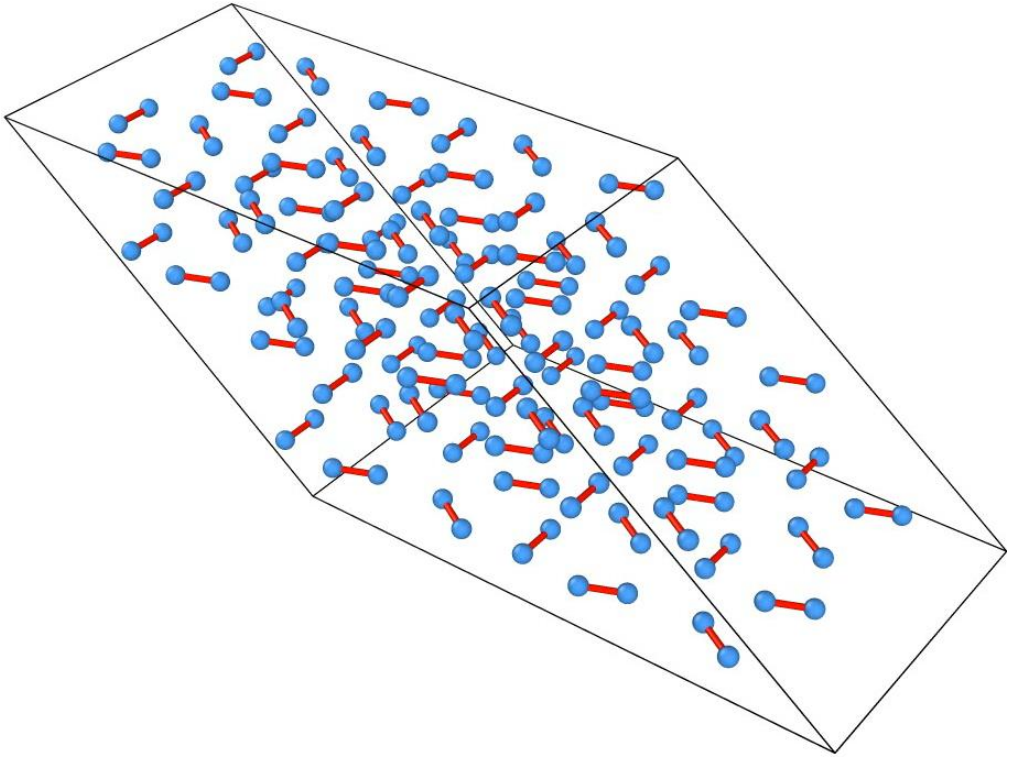

Dependence of pressure on density at T = 100 K
(molecular phase)
P [Mbar]
6
5
4
3
Cmca-4
C2/c
1.1
1.2
1.3
1.4
1.5
1.6
ρ [g/cm3]

MD at density 1.5 g/cm^3



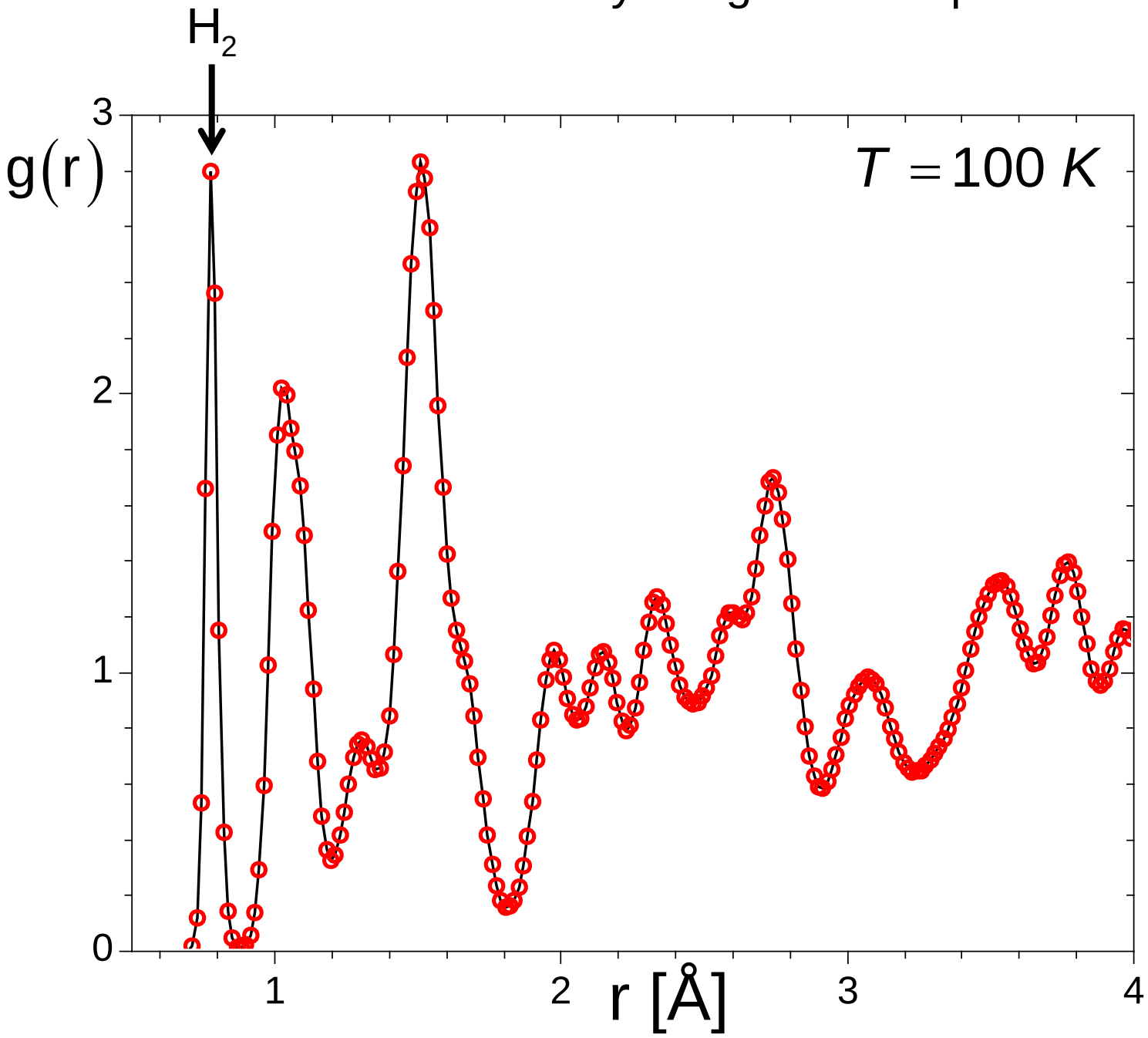






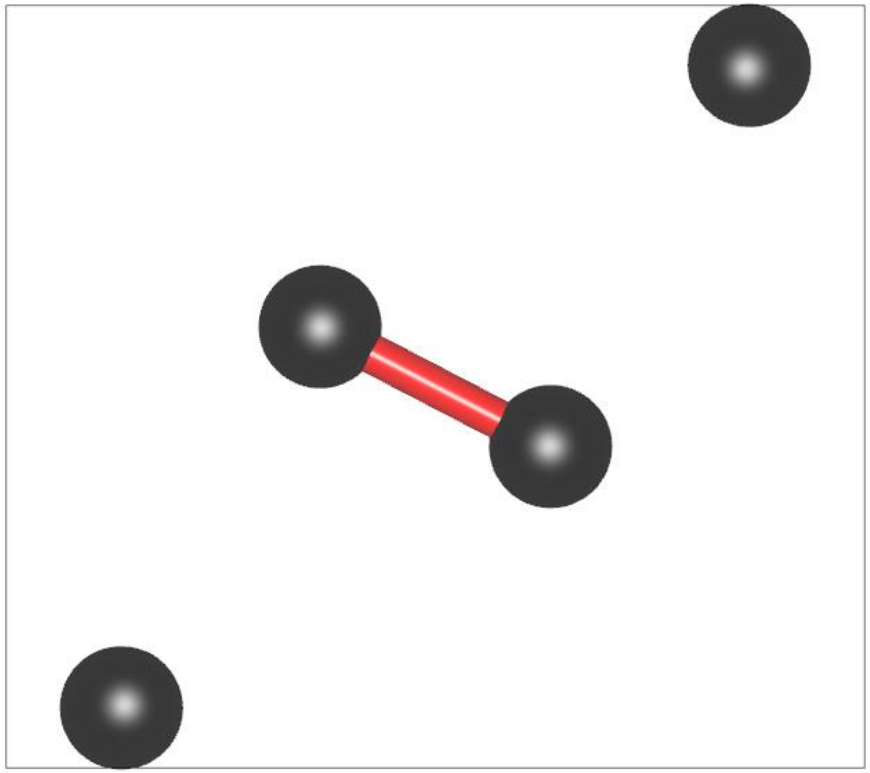
Conductivity at density 1.5 g/cm^3: 830 (Ohm·cm)$^{-1}$

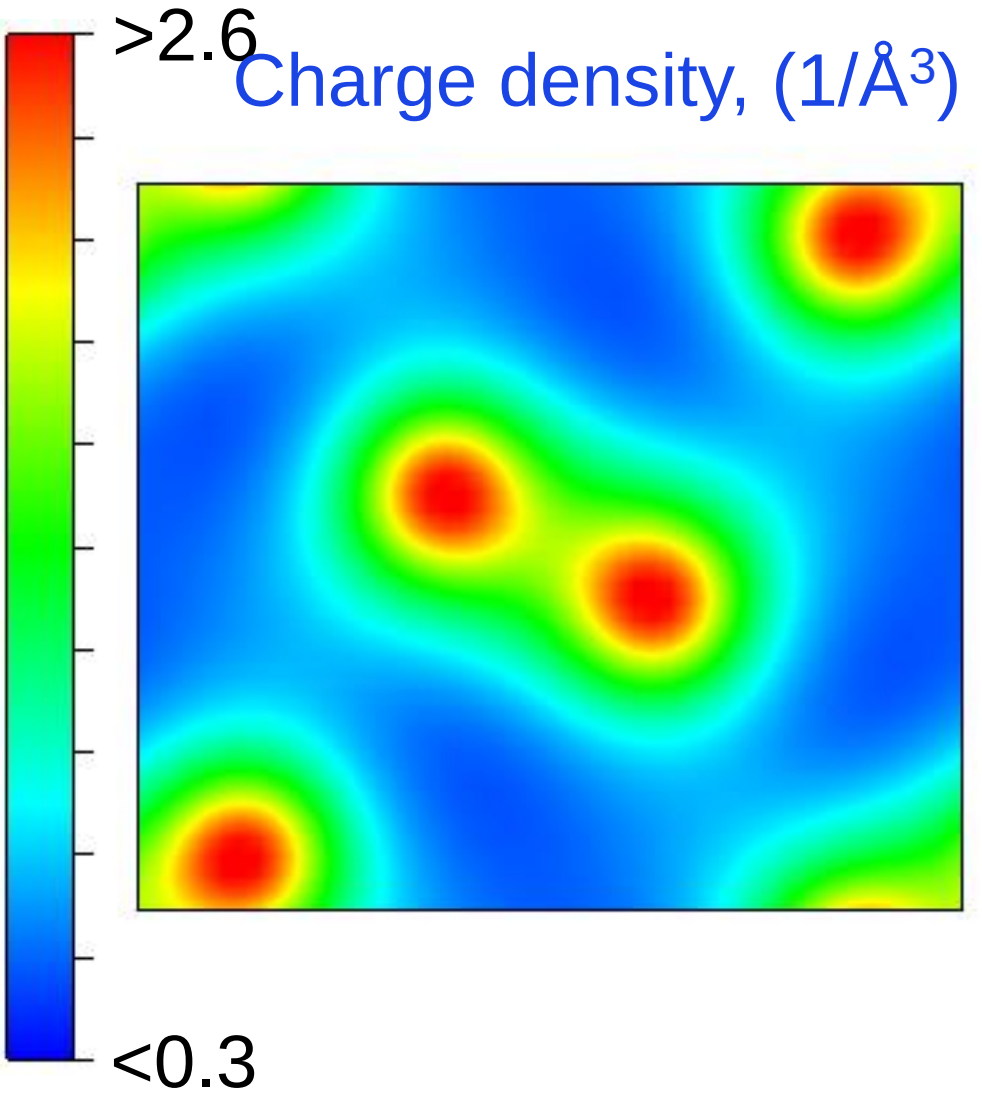
Pair correlation function at density 1.5 g/cm^3 and pressure 568 GPa



Primitive cell and charge density at pressure 568 GPa

Space group: Cmca-4



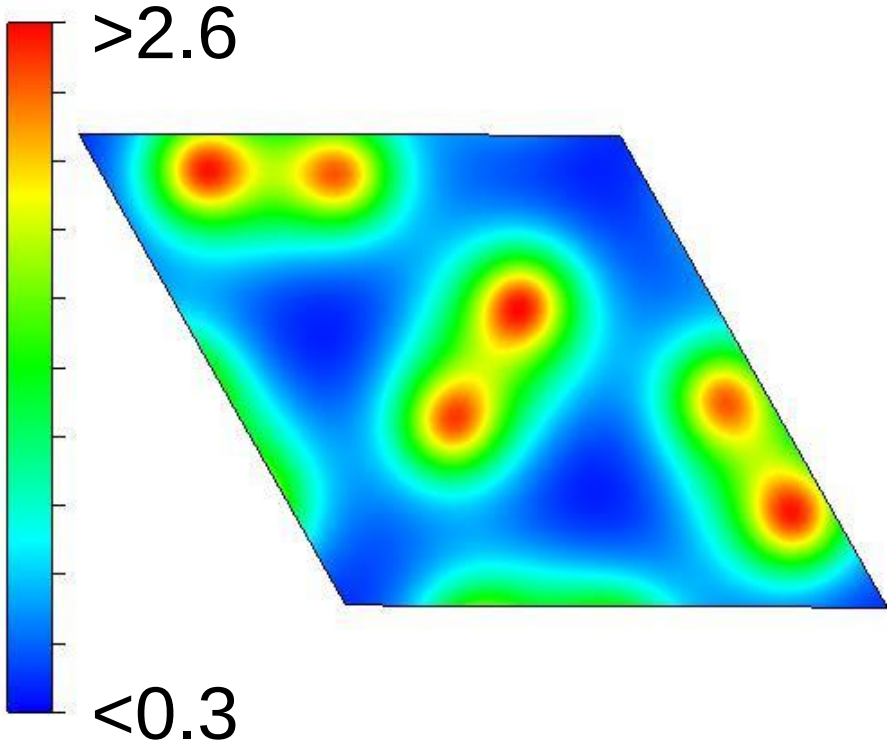


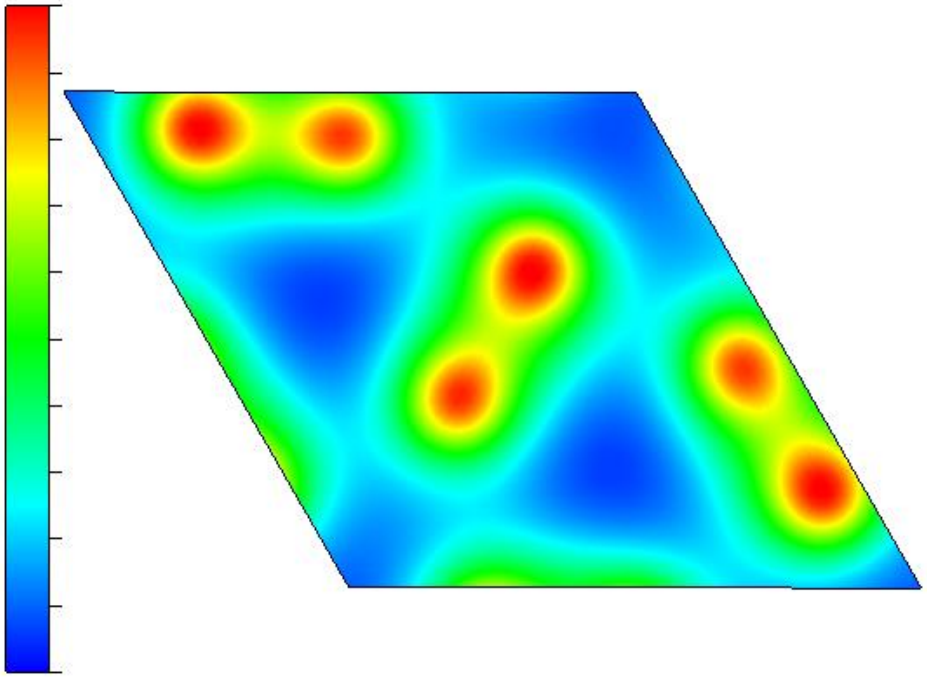
3. Semimetallic states of molecular crystalline hydrogen

Charge density of C2/c structure

P=302 GPa

P = 410 GPa

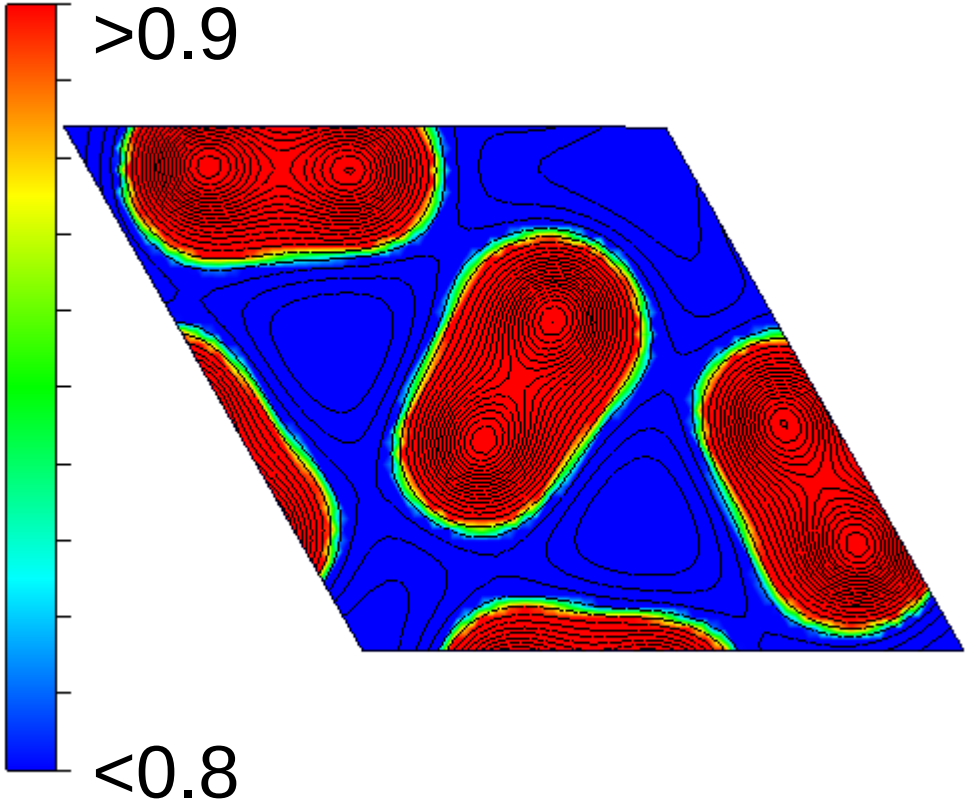


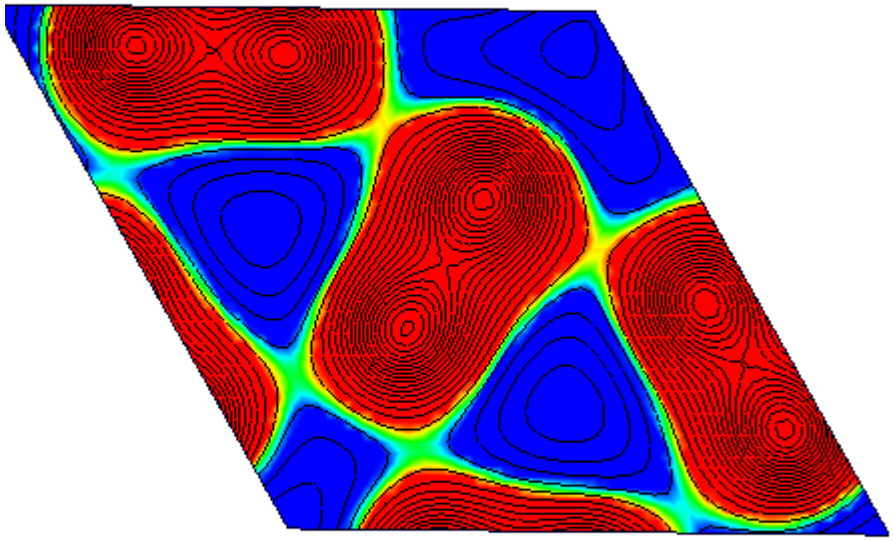


Charge density of C2/c structure

P=302 GPa

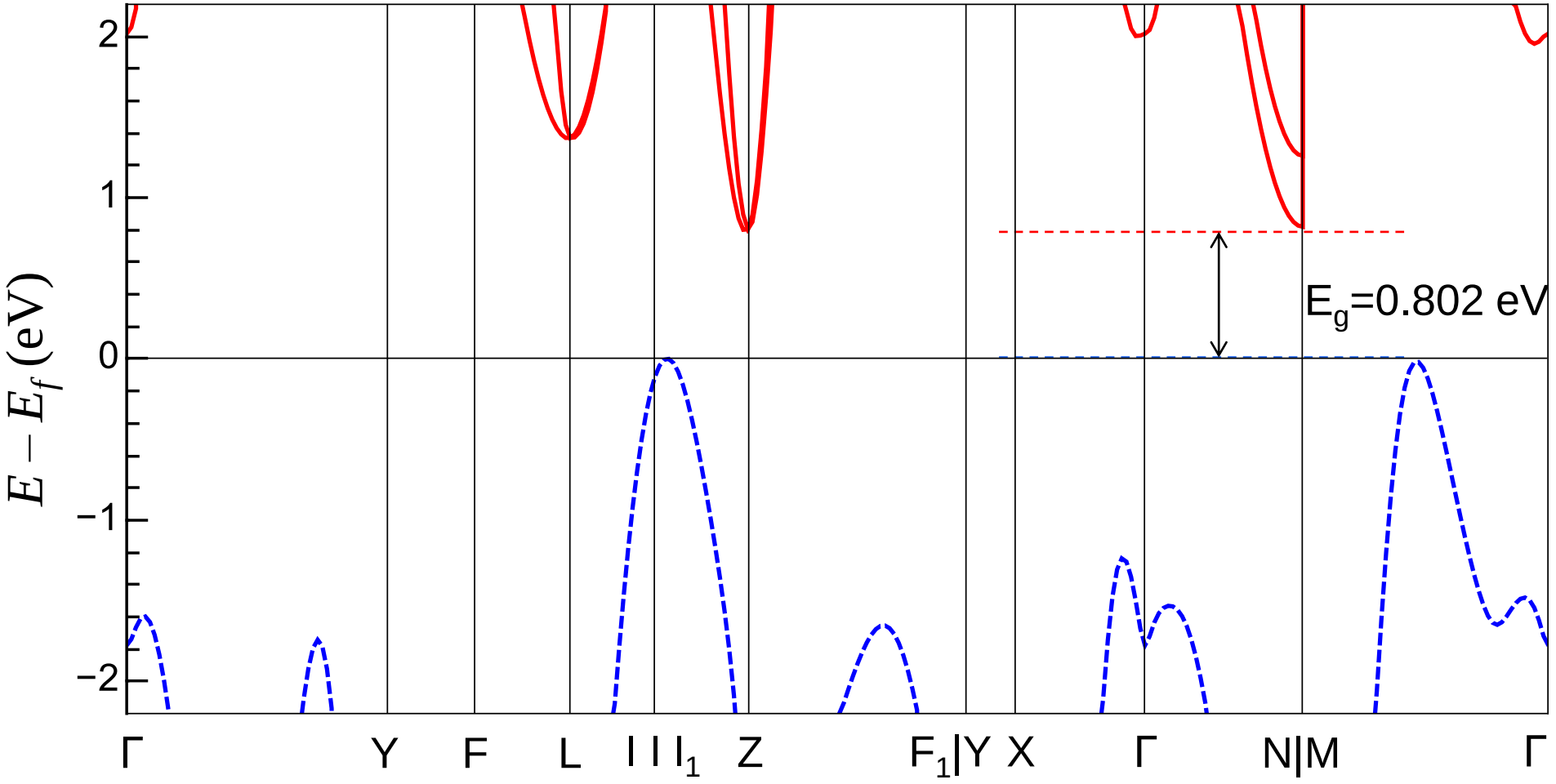
P = 410 GPa





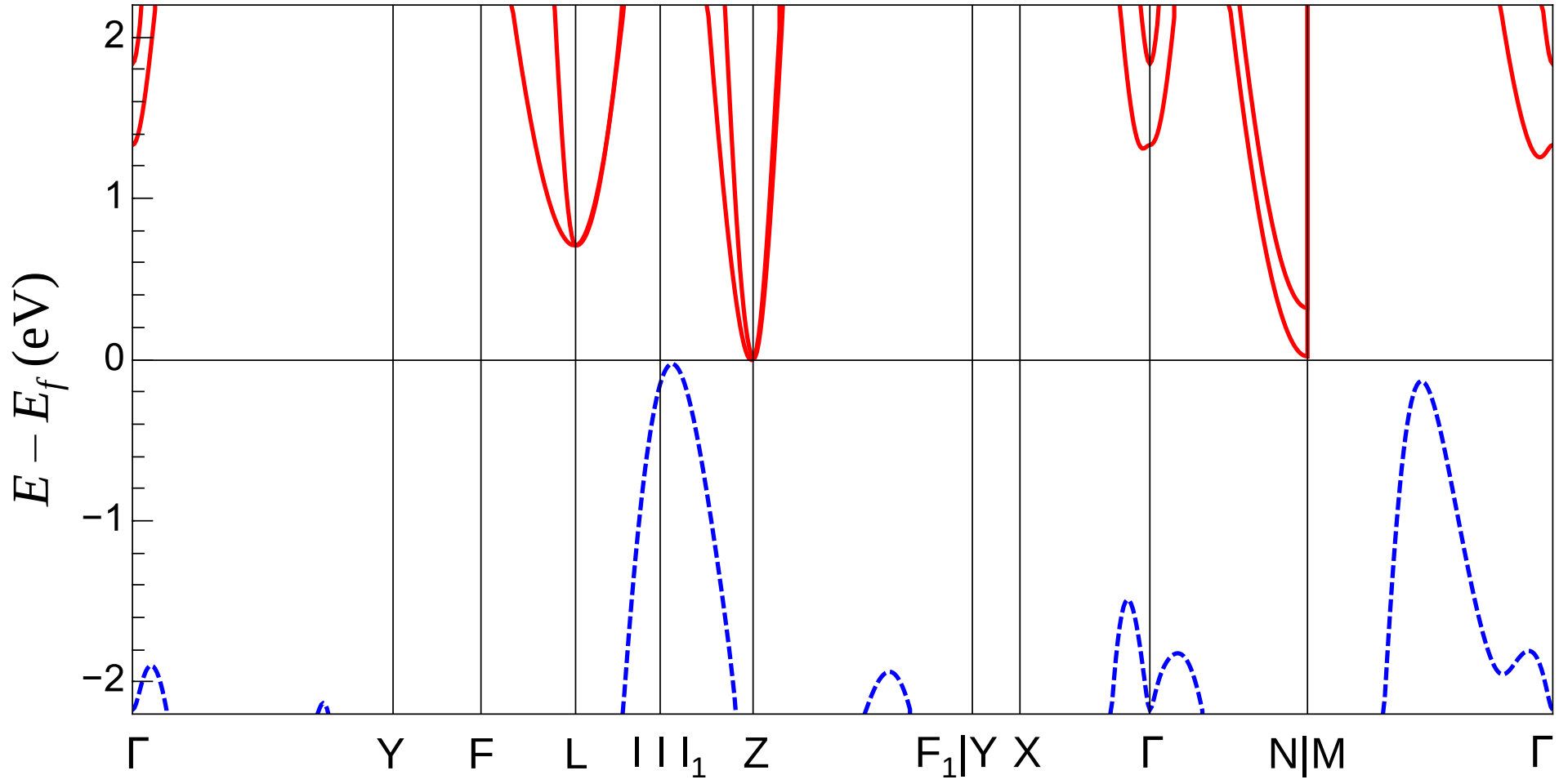
Band structure of C2/c

P=302 GPa



Band structure of C2/c

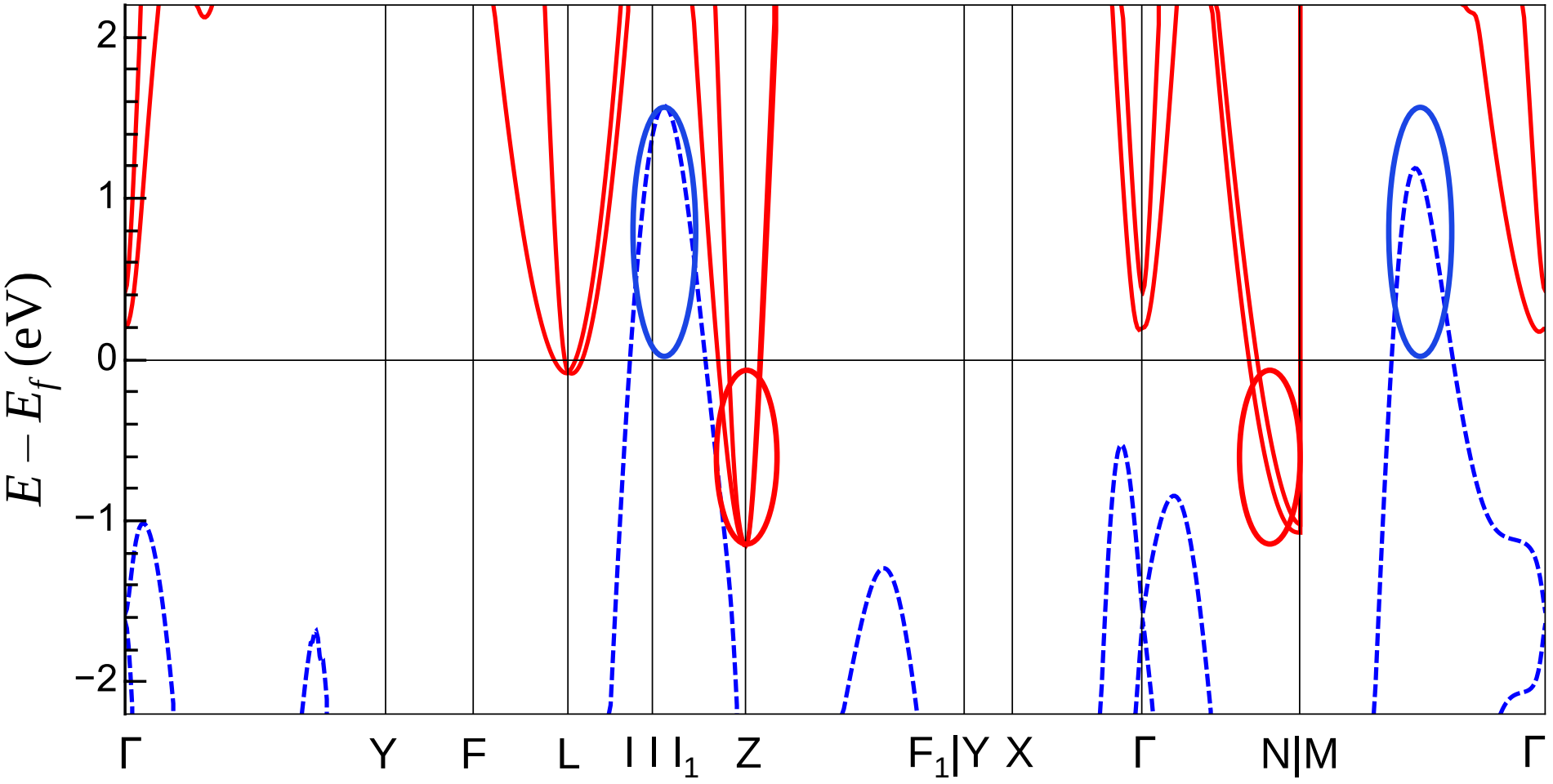
P=361 GPa



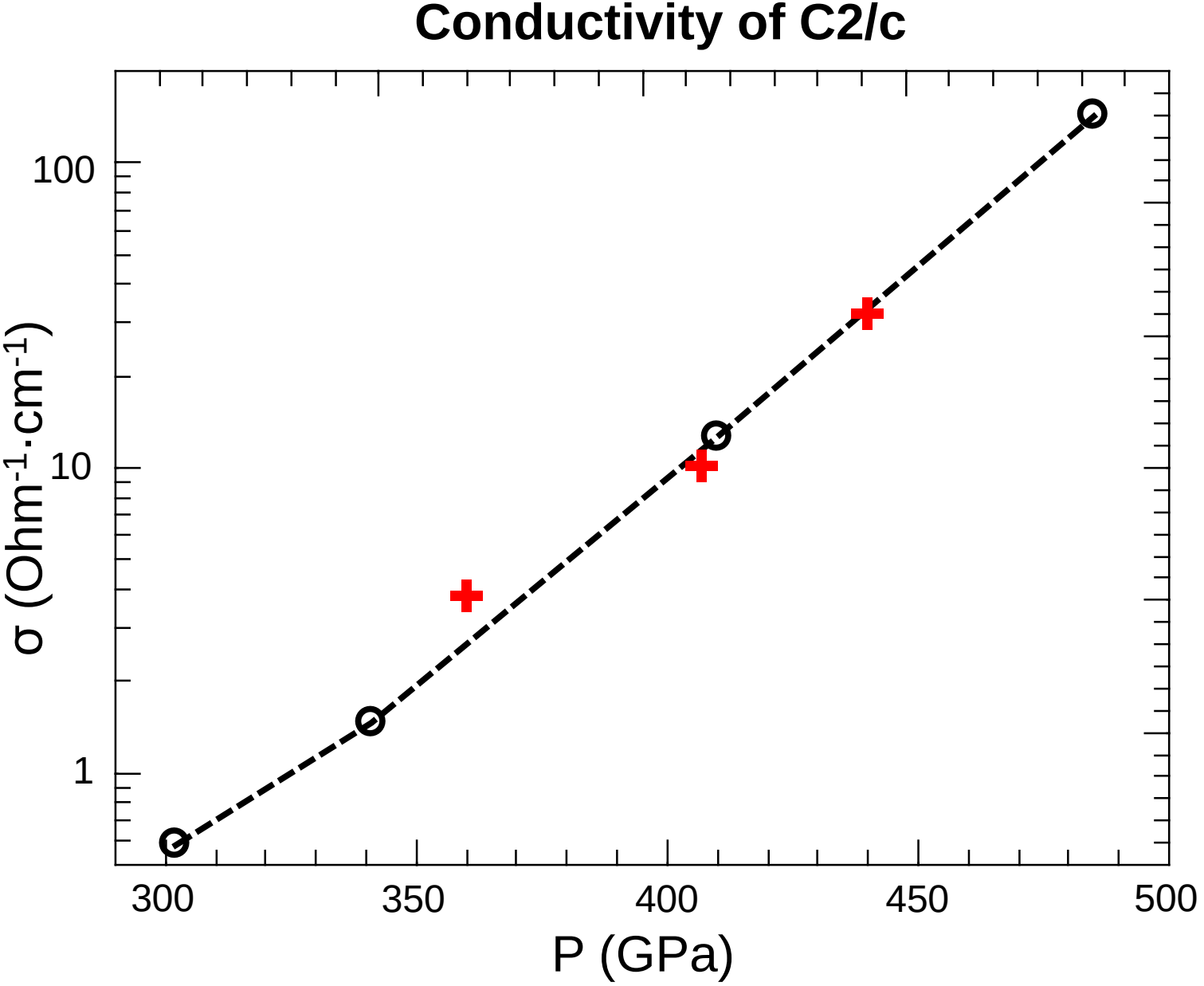
Band structure of C2/c

P=527 GPa

semimetal



Г.Э. Норман, И.М. Саитов Полуметаллические состояния кристаллического молекулярного водорода при высоких давлениях // Письма в ЖЭТФ. 2020. Т. 111. №3. С. 175 – 180.



Г.Э. Норман, И.М. Саитов // Письма в ЖЭТФ. Февраль 2020.

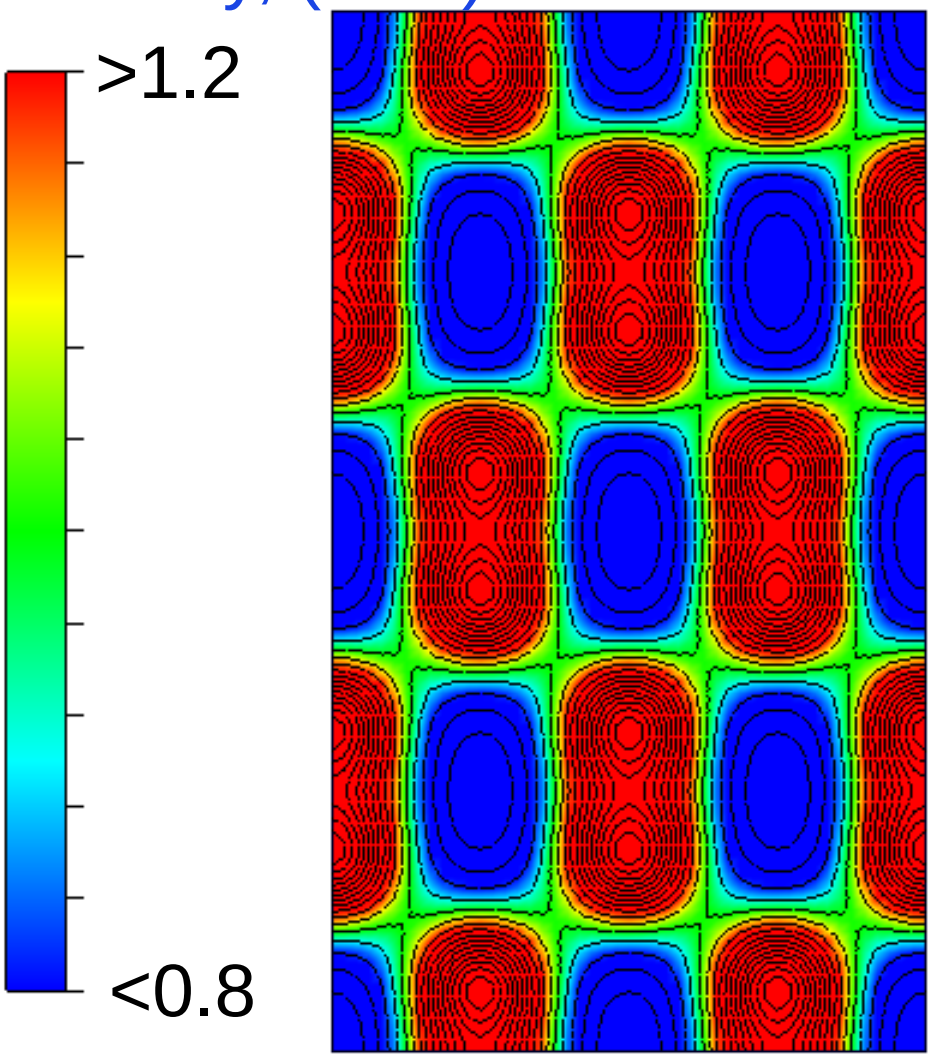
M. I. Eremets et al // Nature Physics. September 2019.

4. Metallic states of molecular crystalline hydrogen

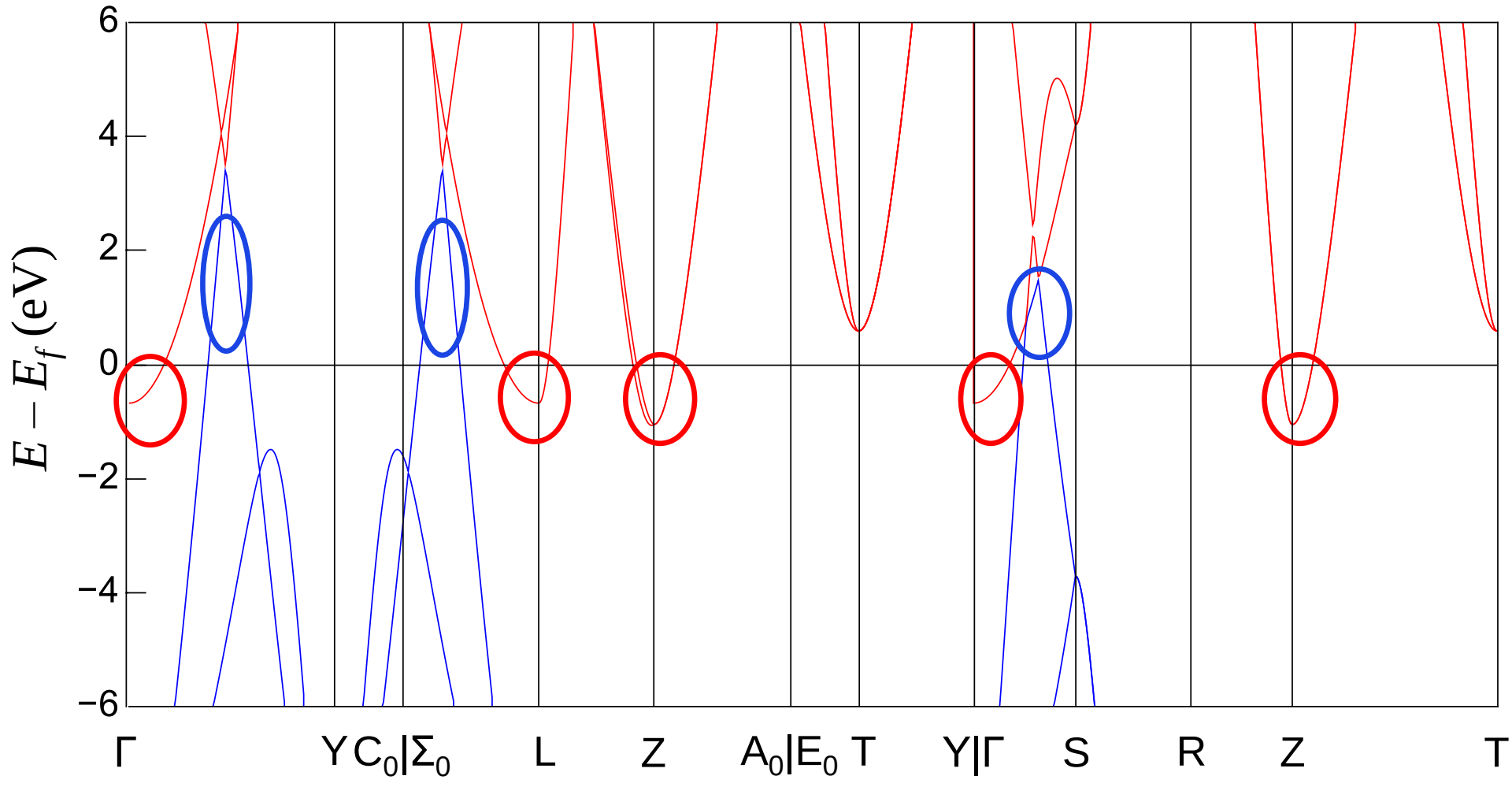
Charge density of Cmca-4 structure

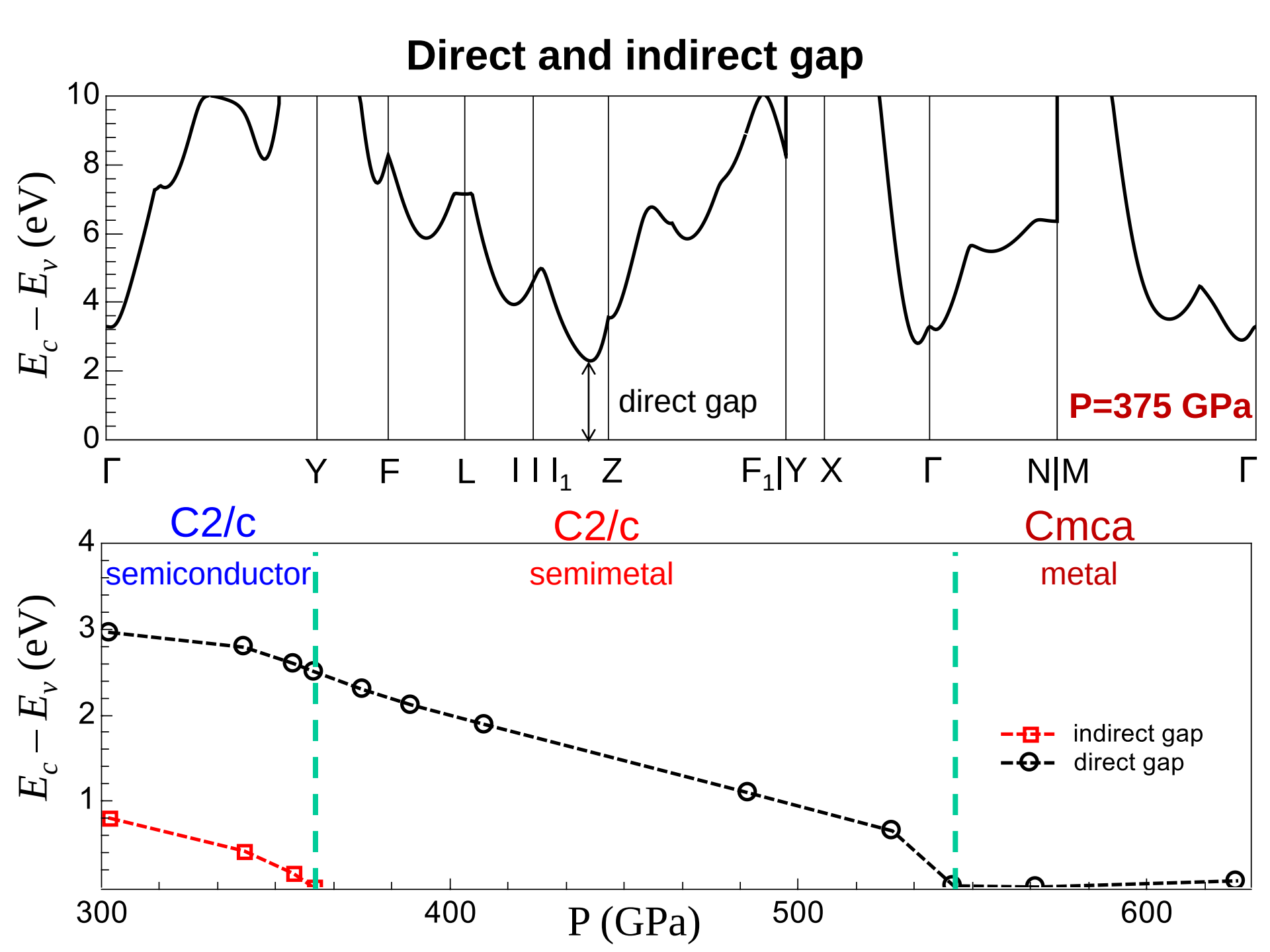
P=626 GPa

Charge density, (1/Å^3)

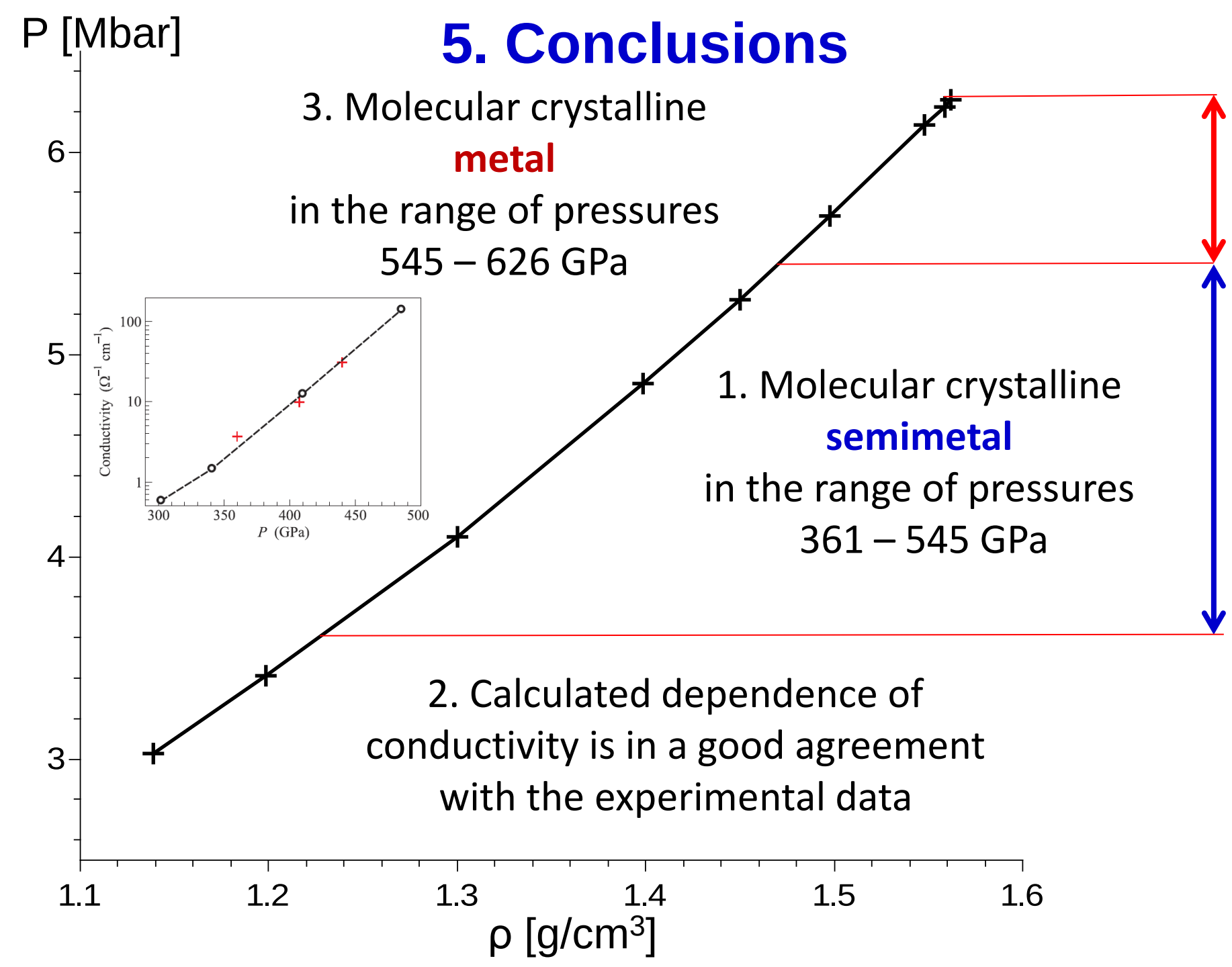


Band structure of Cmca




Direct and indirect gap
$E_c - E_v$ (eV)
10
8
6
4
2
0
direct gap
P=375 GPa
Γ
Y
F
L
I I I$_1$
Z
F$_1$|Y
X
Γ
N|M
Γ
C2/c
semiconductor
C2/c
semimetal
Cmca
metal
4
3
2
1
indirect gap
direct gap
300
400
500
600
P (GPa)

5. Conclusions



3. Molecular crystalline **metal** in the range of pressures 545 – 626 GPa

1. Molecular crystalline **semimetal** in the range of pressures 361 – 545 GPa

2. Calculated dependence of conductivity is in a good agreement with the experimental data