Ab-initio study of $Ti_3Si_{0.5}Ge_{0.5}C_2$ under pressure up to 80 GPa

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Outline

1. Max Phases

2. Computational method

3. Results

   -Structural properties: energy volume, cell parameters

   -Electronic porperties: Bands structure, DOS

4. Conclusions

MAX phases

Ternary layered compounds

M_{N+1} A X_N (N=1 to 3)

M_{N+1}	A	X_N
early transition metal Ti Nb Hf	group III or IV Al, Si Ga, Ge In, Sn	Group IV or V C, N

Ex.: Ti_2AlC, Ti_3SiC_2 , Ti_4AlN_3

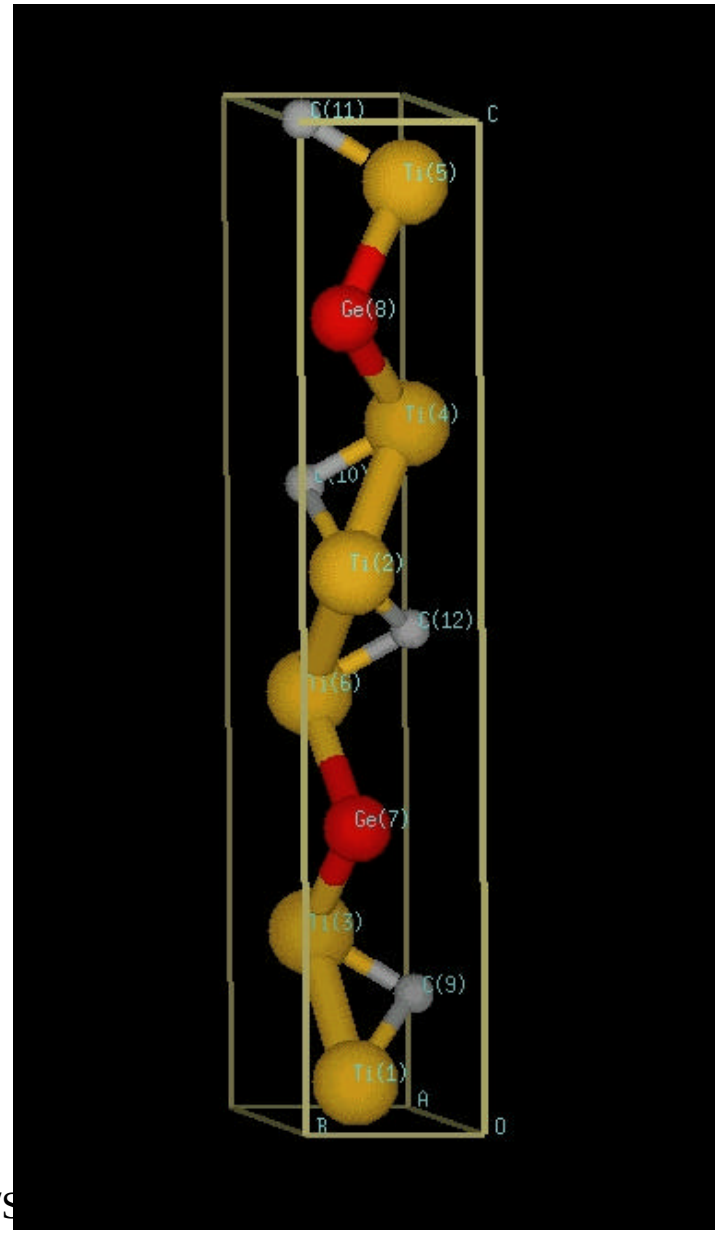
MAX phases properties

Best attributes of metals and ceramics

Like metals:
Thermal and electrical conductors
Readily machinable
Plastic at high temperatures

Like ceramics:
Elastically rigid
Lightweight
Mantain their strengths at high temperature

M_3AX_2 unit cell



- Hexagonal cell,

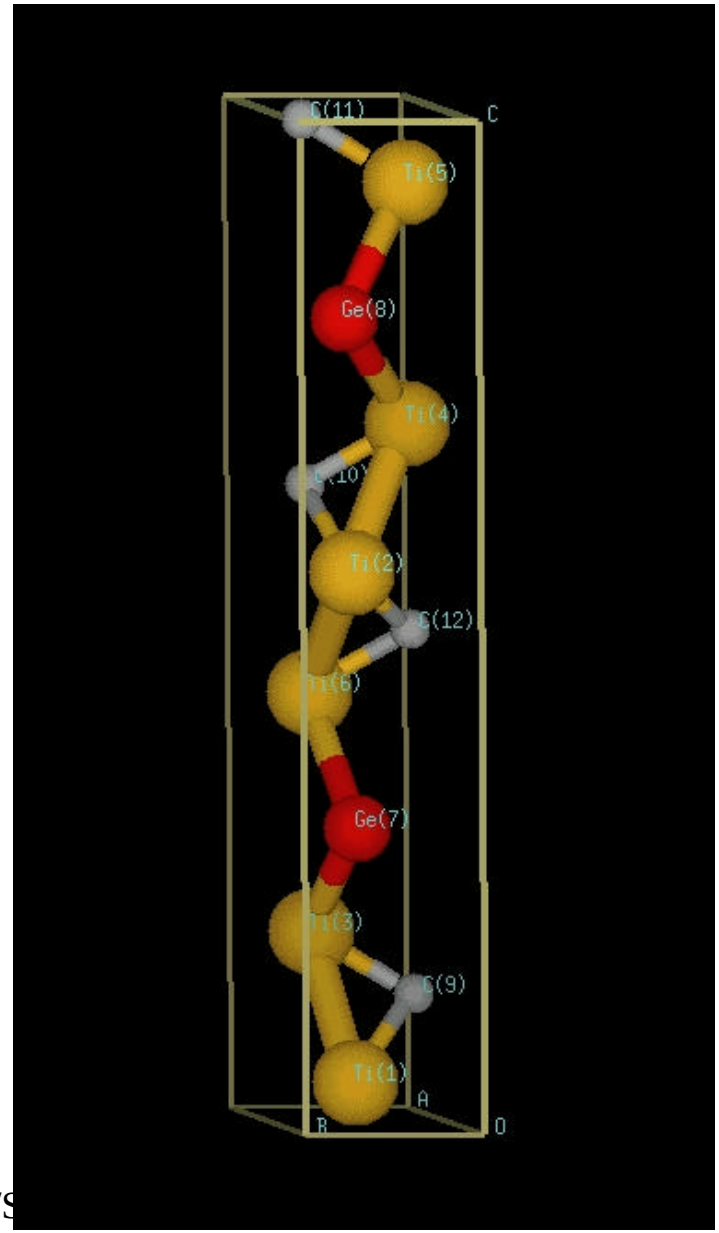
a ~ 3 Å

c ~ 17 Å

- Two formula unit per unit cell

- Like TiC, but interleaved with layers of A atoms

$Ti_3Si_{0.5}Ge_{0.5}C_2$: structrure



- Hexagonal cell,

a ~ 3.079 Å

c ~ 17.77 Å

- Bulk Modulus

B=183 +/- 4 GPa

(APL, Manoun et al, (2004)).

Computational method

-DFT with LDA

-SIESTA code:
strictly-localized numerical pseudoatomic orbital

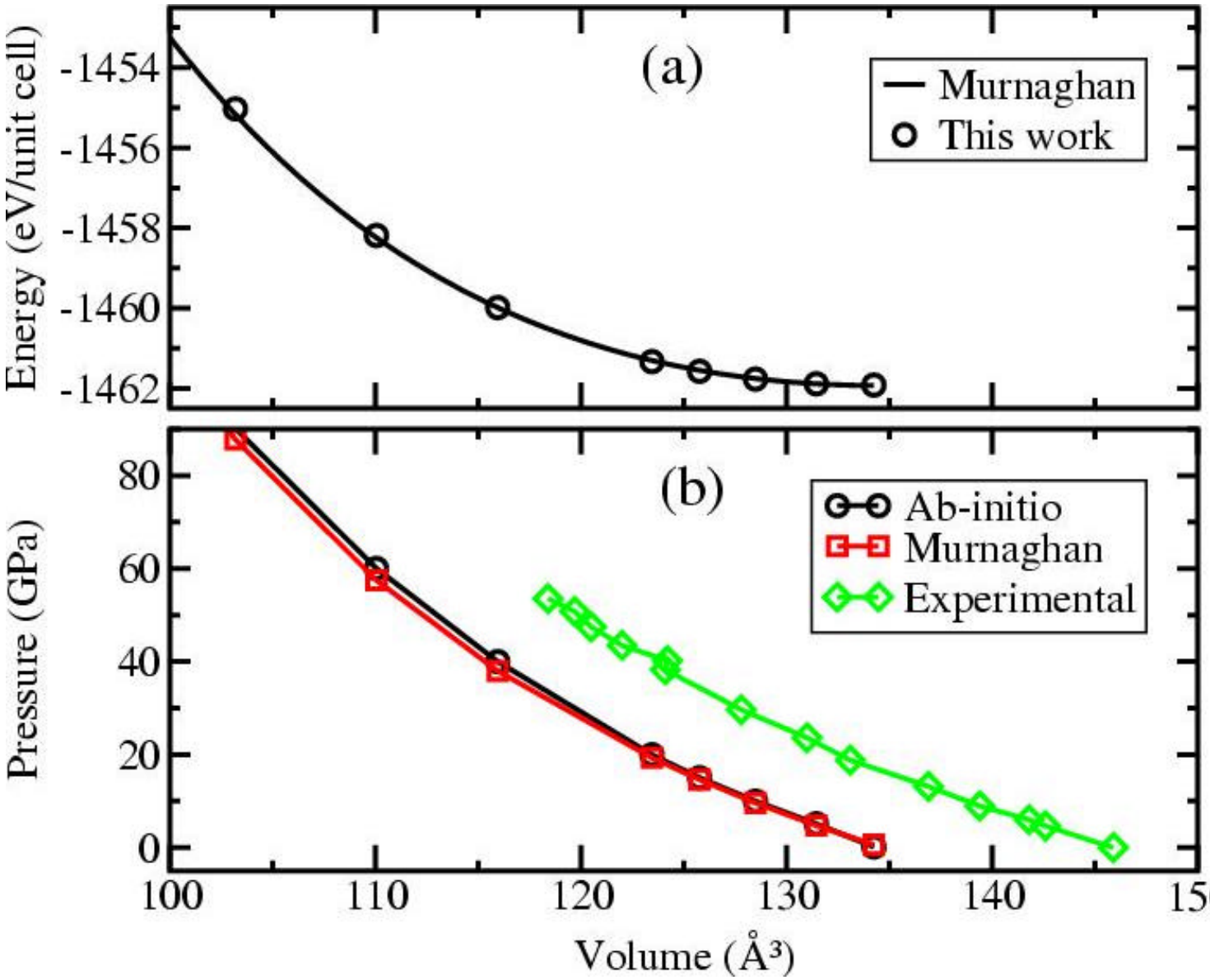
-Norm-conserving pseudopotential, fully separable form

-Double zeta single polarized (DZP) basis set

-7x7x2 k points in the Brillouin zone (Monkhorst-Pack mesh)

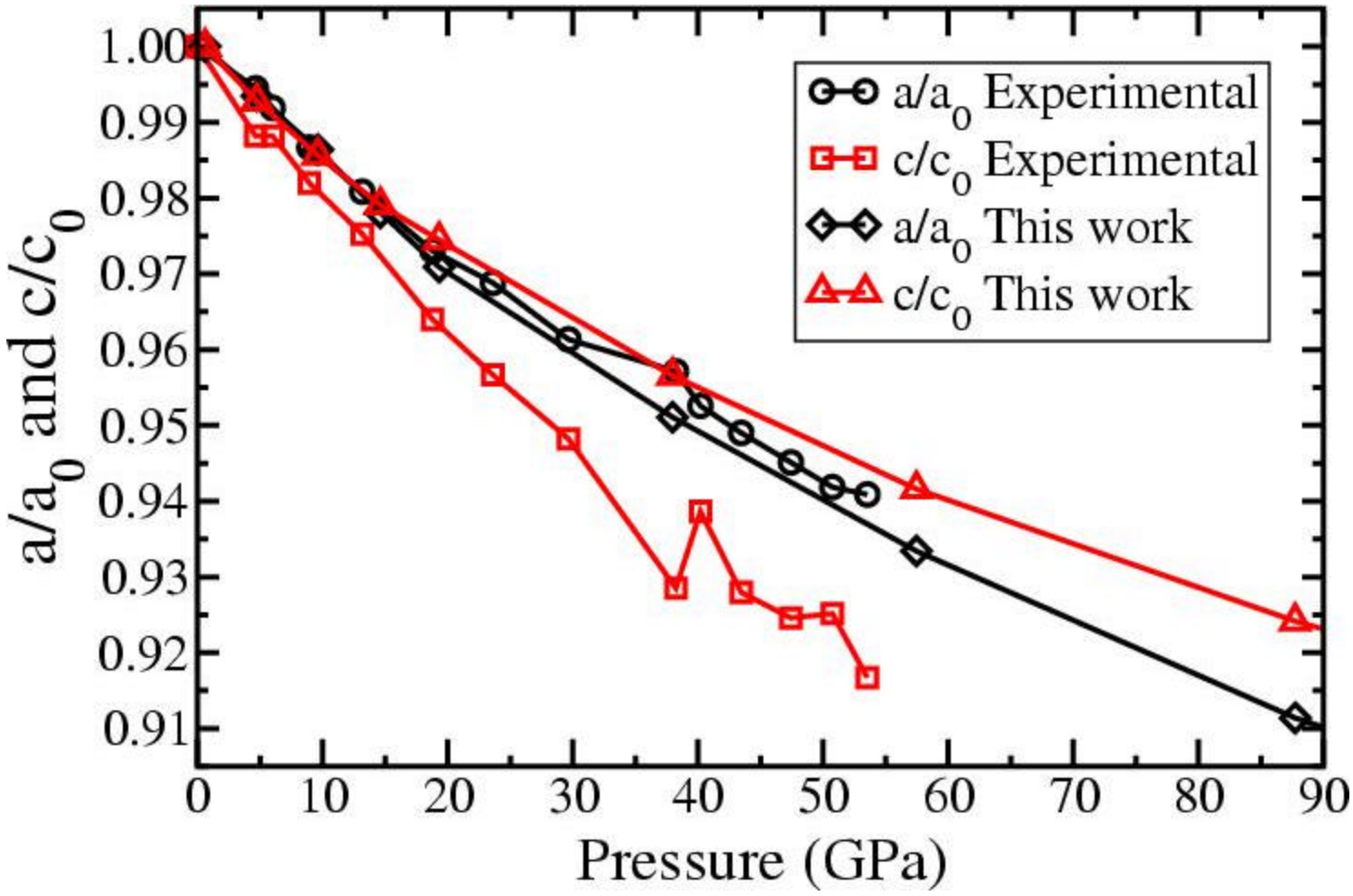
-For high pressure, hydrostatic pressure was applied, using variable cell approach within Parrinello-Rahman method.

Energy v/s volume



B=185 GPa

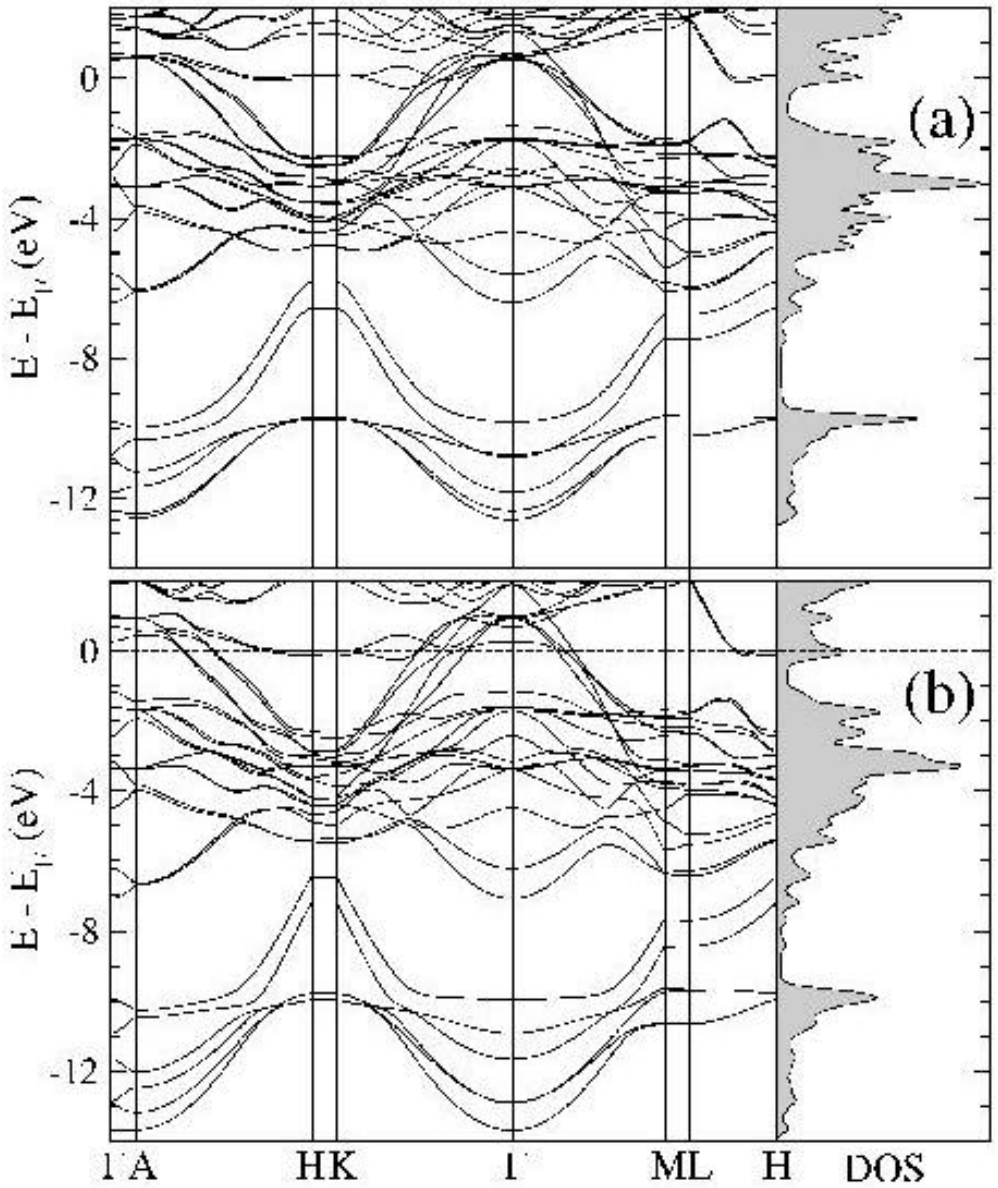
Lattice parameters v/s pressure



Structural changes under pressure

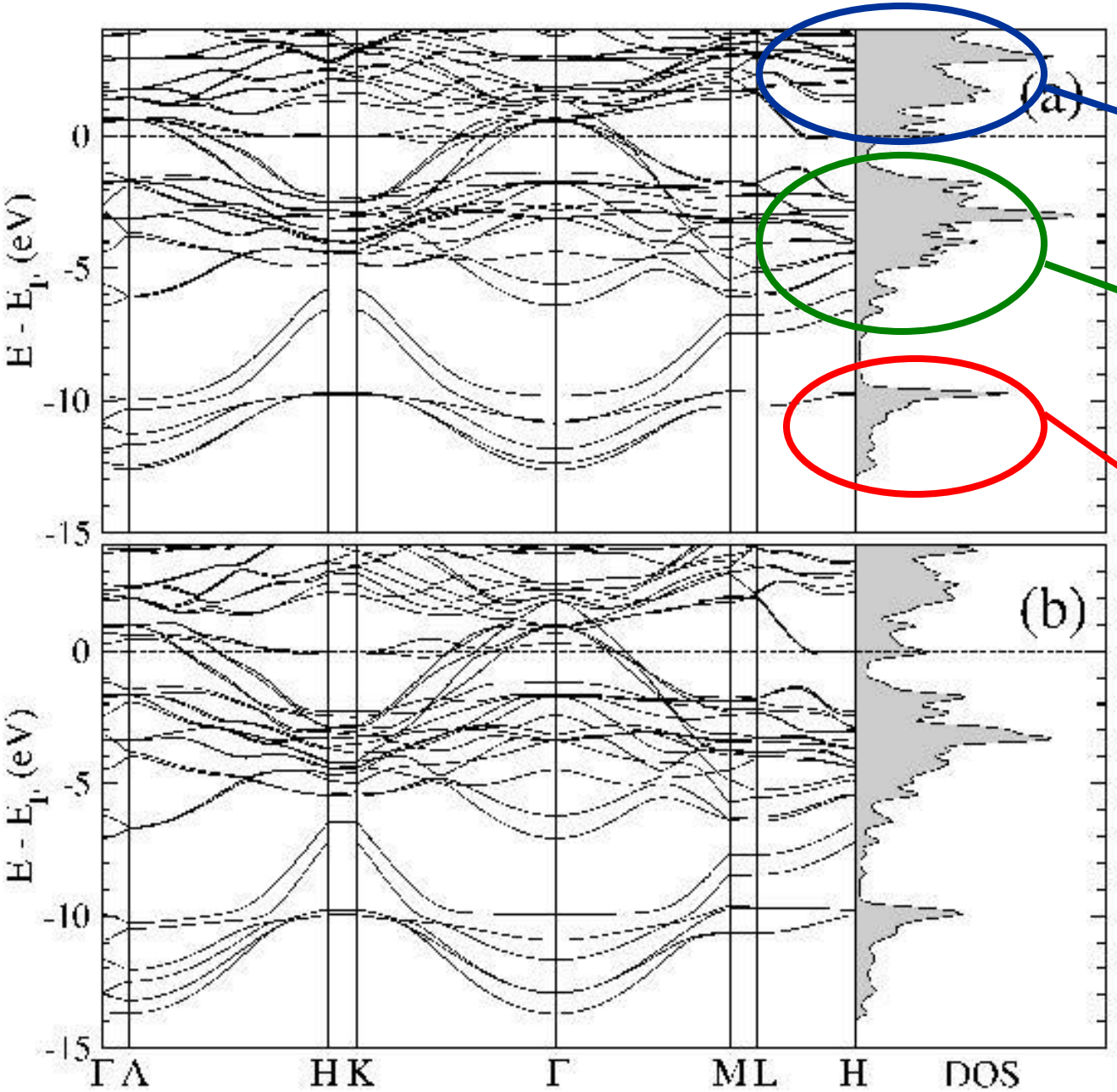
	0 GPa	80 GPa
Distances		
Ti-Ge	2.68	2.42 (-10%)
Ti-Si	2.63	2.38 (-9.6%)
Ti-C	2.11	1.93 (-8%)
Angles		
Ti-Ge-Ti	99.4	98.8
Ti-Si-Ti	97.9	96.4
Ti-C-Ti	87.9	89.4

Bands structure at 0 and 80 GPa



Bands structure almost the same

Dos: the density of states at the fermi level decrease

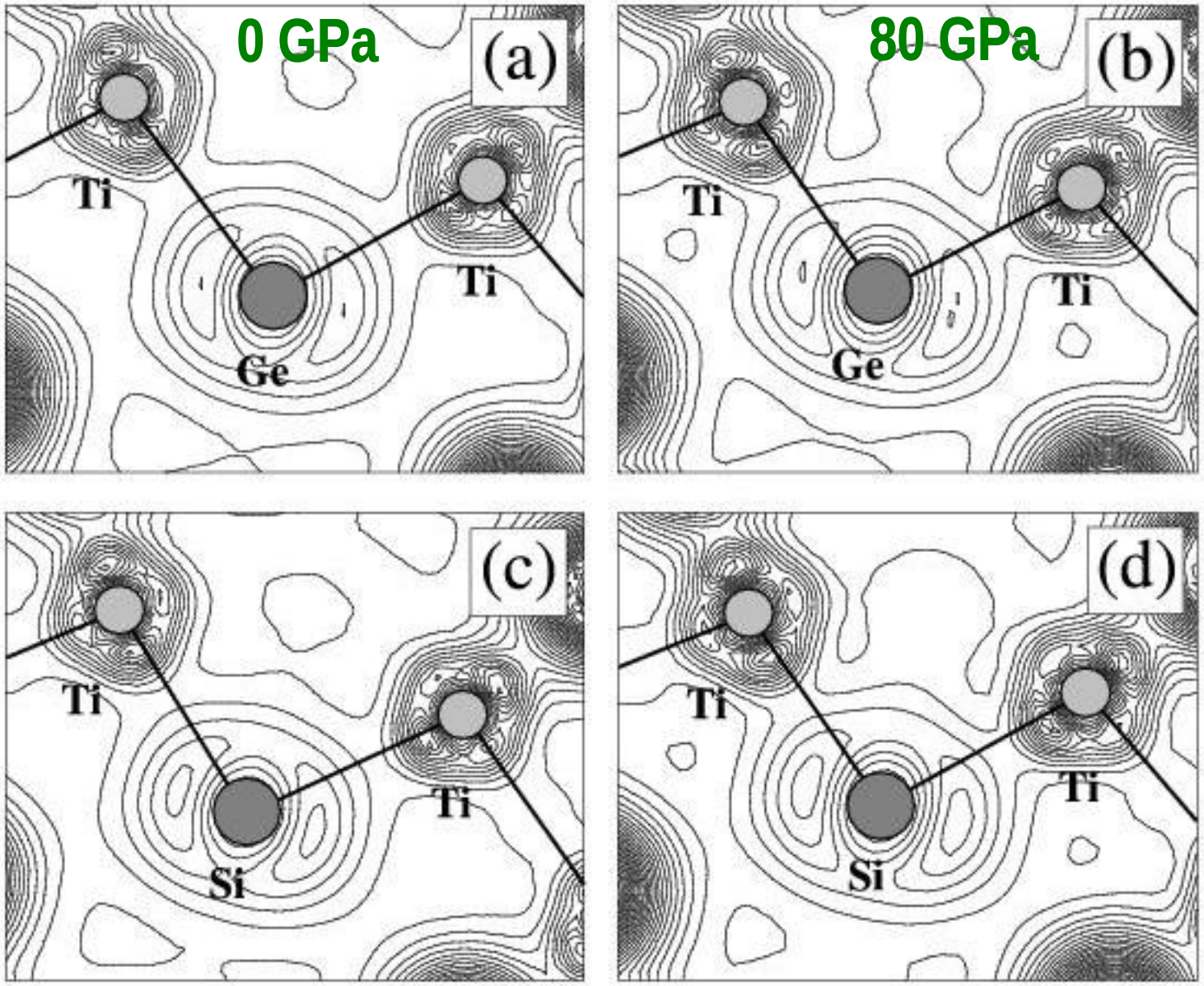


Ti 3d

Ti 3d, C 2p,
Si, Ge 3p

C 2s, Si 3s

Charge density



Conclusion

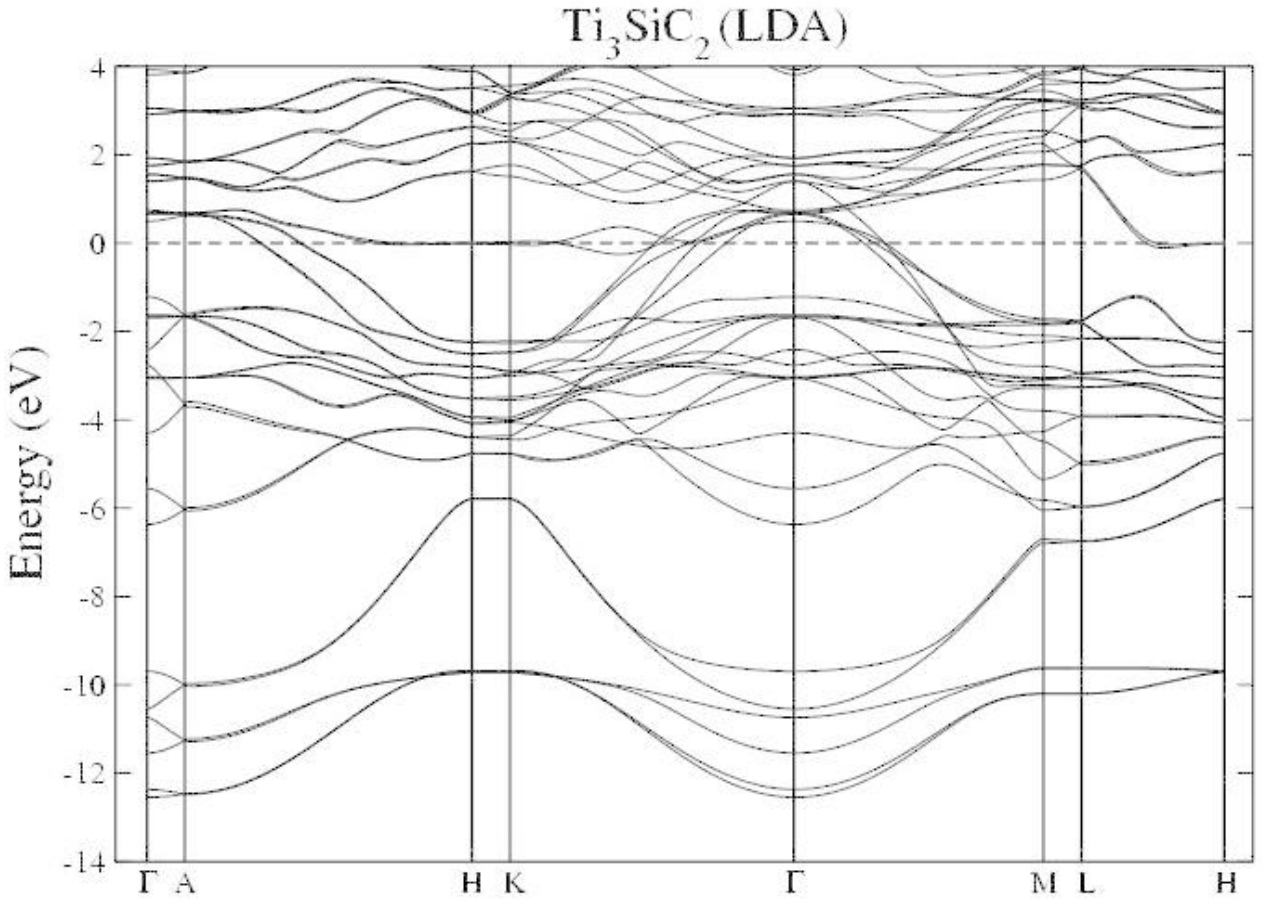
1) There is no major changes up to 80 GPa.
It is very likely that the good properties
at O GPa remain under pressure.

2) There is almost no anisotropy under compression,
in contrast to the experiment.

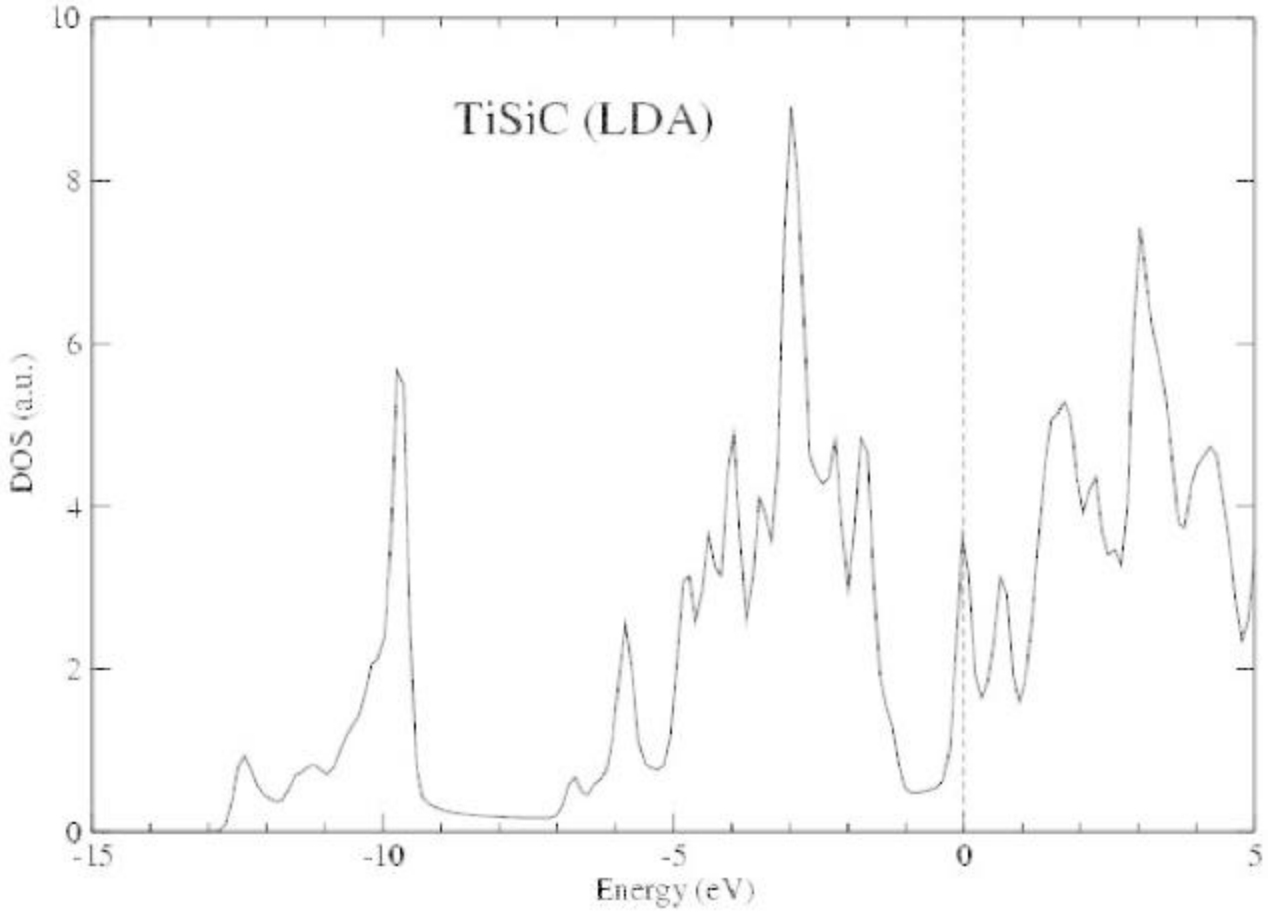
3) Physical properties which depend on the density of
states at fermi level could change, because the
decrease of DOS at the fermi level under pressure.

Acknowledgments: Grant from Fondecyt, Chile.
Computer time of MAIDROC at FIU.

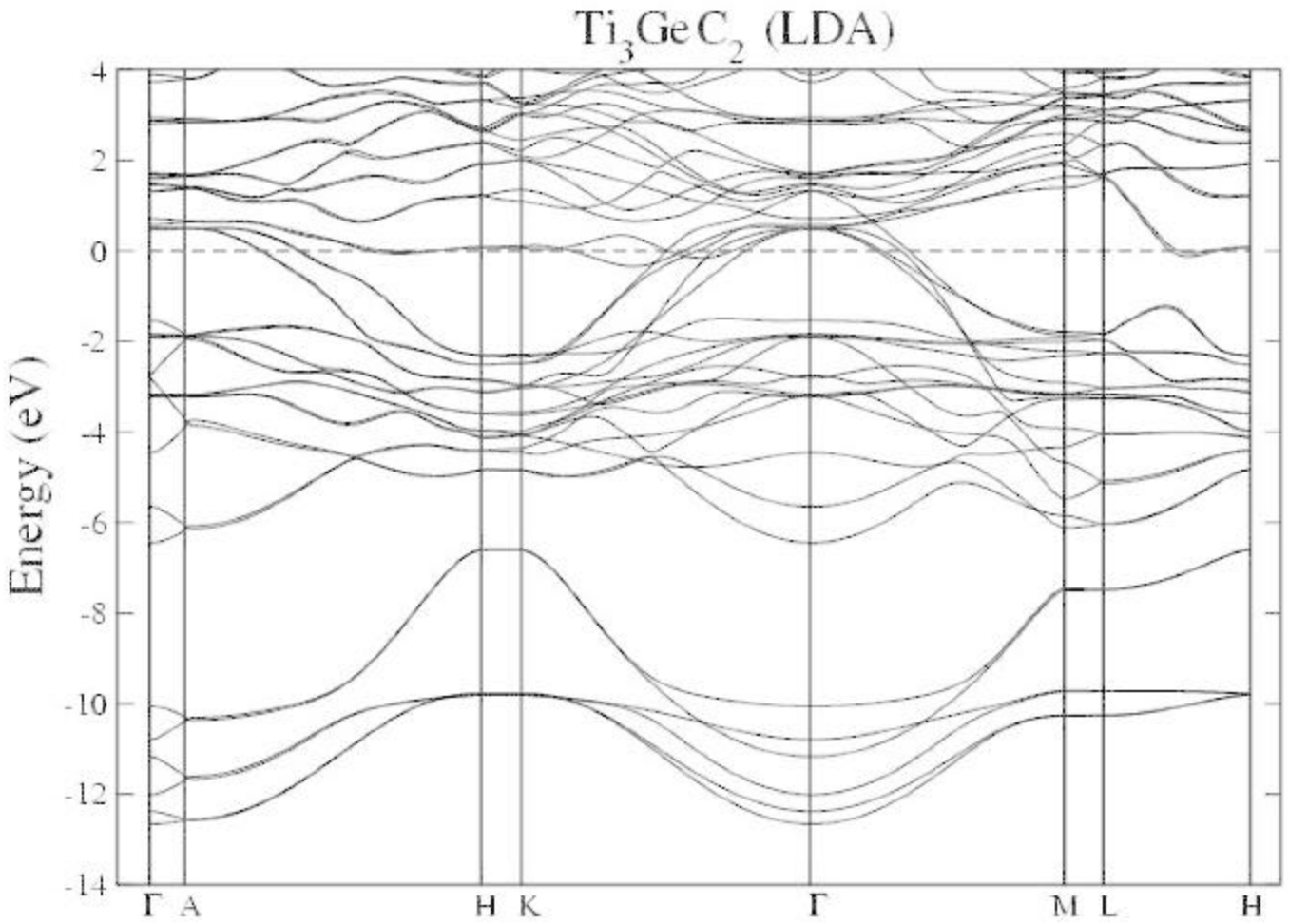
Ti_3SiC_2 : band structrure



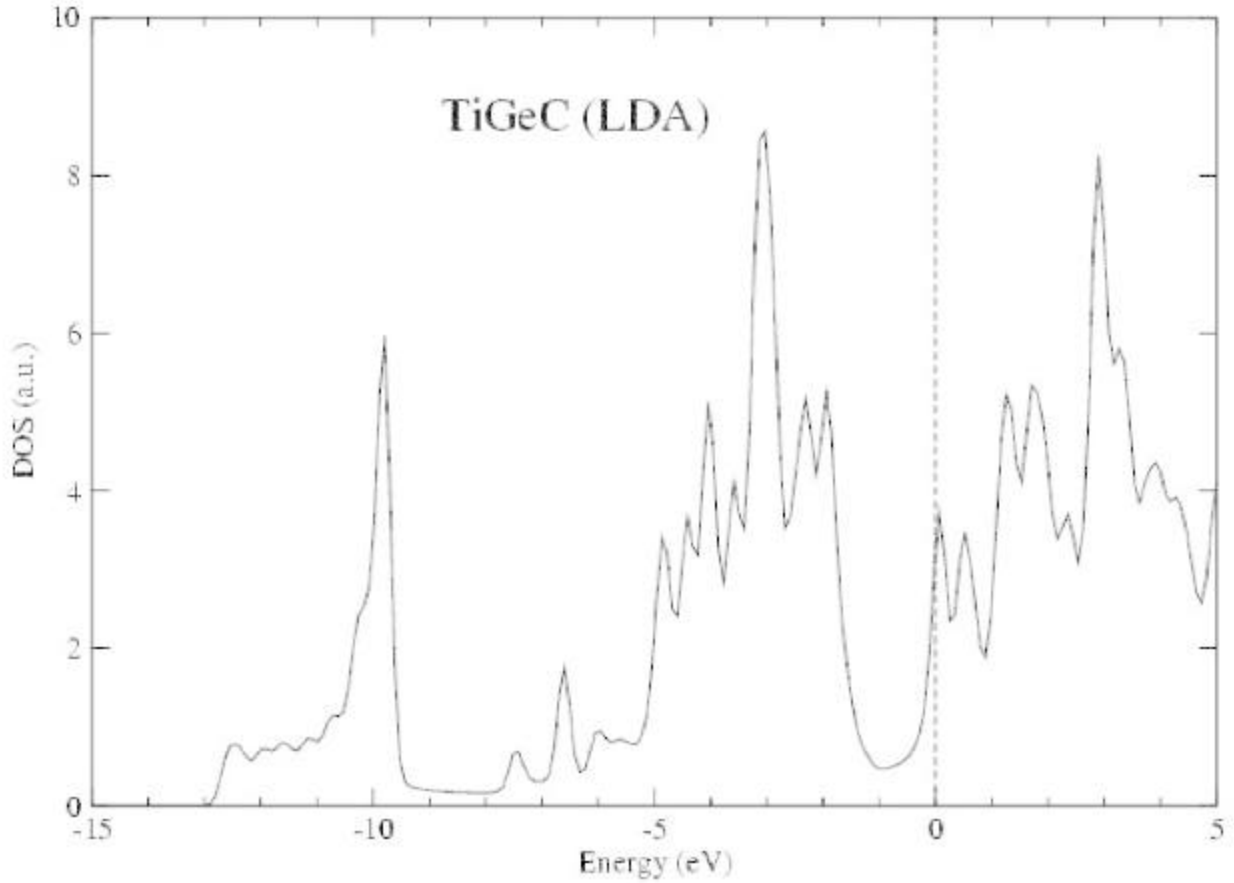
Ti_3SiC_2 : dos



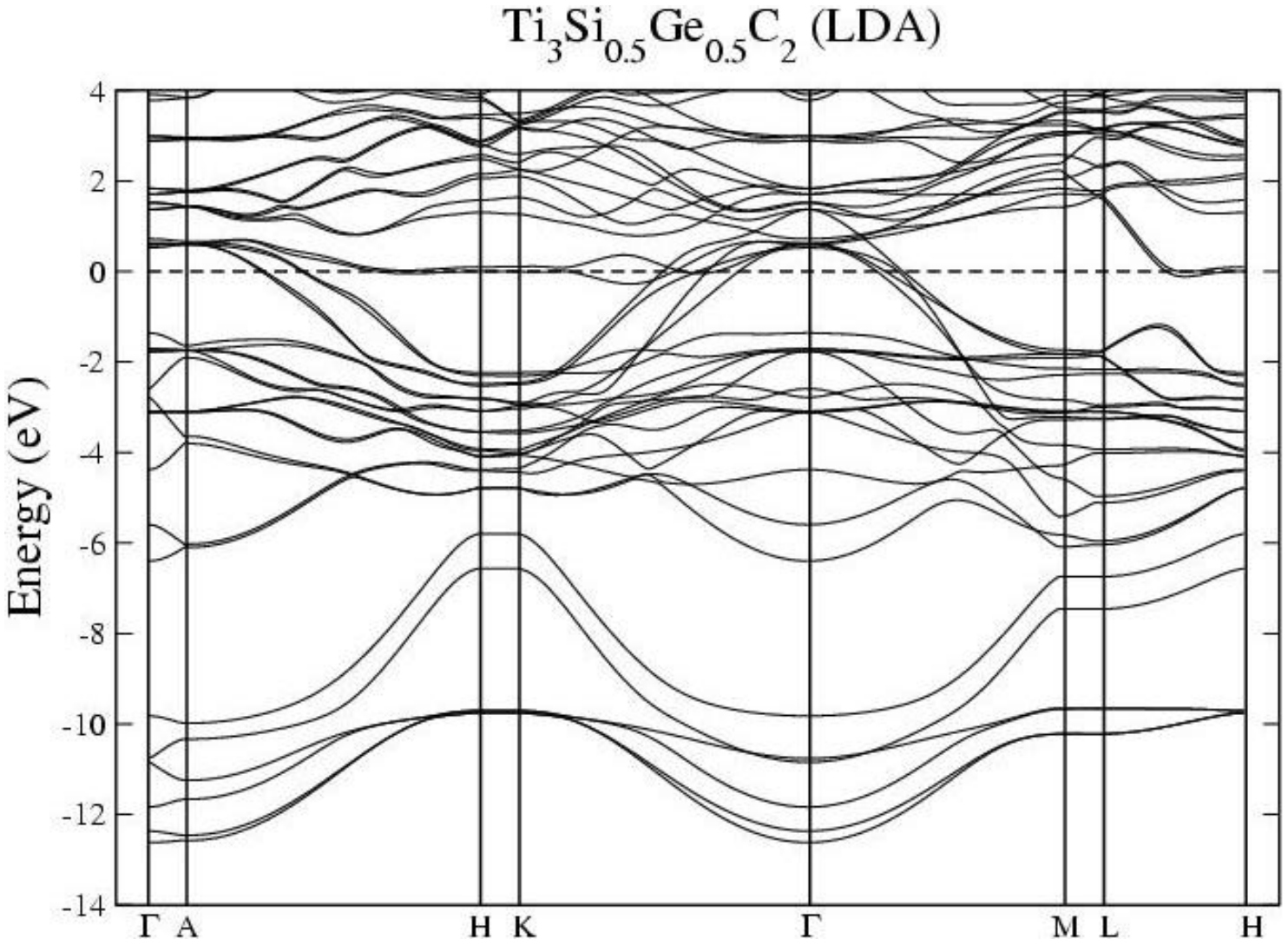
Ti_3GeC_2 : band structrure



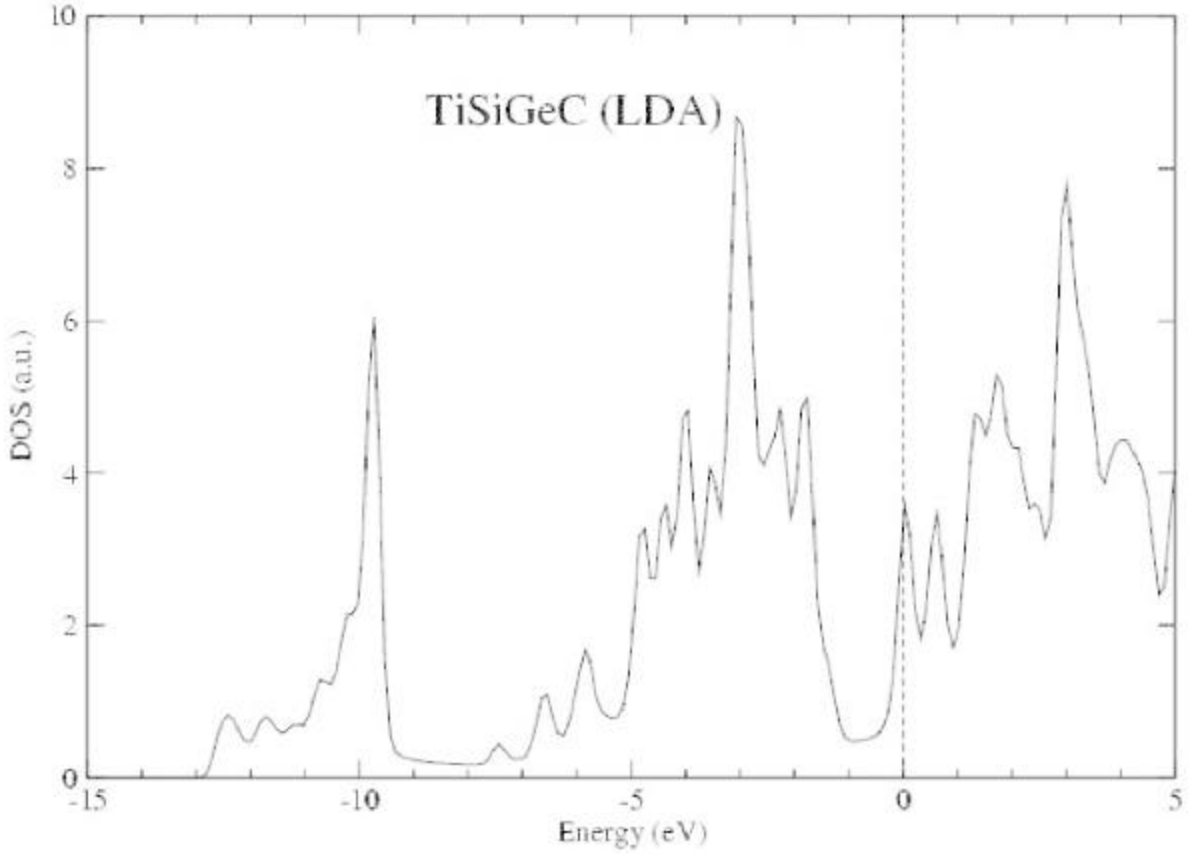
Ti_3GeC_2 : dos



$Ti_3Si_{0.5}Ge_{0.5}C_2$: band structrure



$Ti_3Si_{0.5}Ge_{0.5}C_2$: dos



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Ti-Ti	2.88	2.72 (-5%)
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