Materials at terapascal pressures

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Density Functional Theory Calculations

Need an accurate quantum mechanical description of the inter-atomic bonding

Must evaluate energies, forces and stresses thousands of times

CASTEP code, plane wave basis, ultrasoft pseudopotentials

Standard Generalized Gradient Approximation (PBE-GGA) for the exchange-correlation energy

Terapascal pressures

1 GPa $\simeq 10^4$ atmospheres

Pressure at the centre of the Earth $\simeq$ 350 GPa $=$ 0.35 TPa

Pressure at the centre of Jupiter $\simeq$ 7 TPa

Pressures at the centres of large exoplanets up to 100 TPa

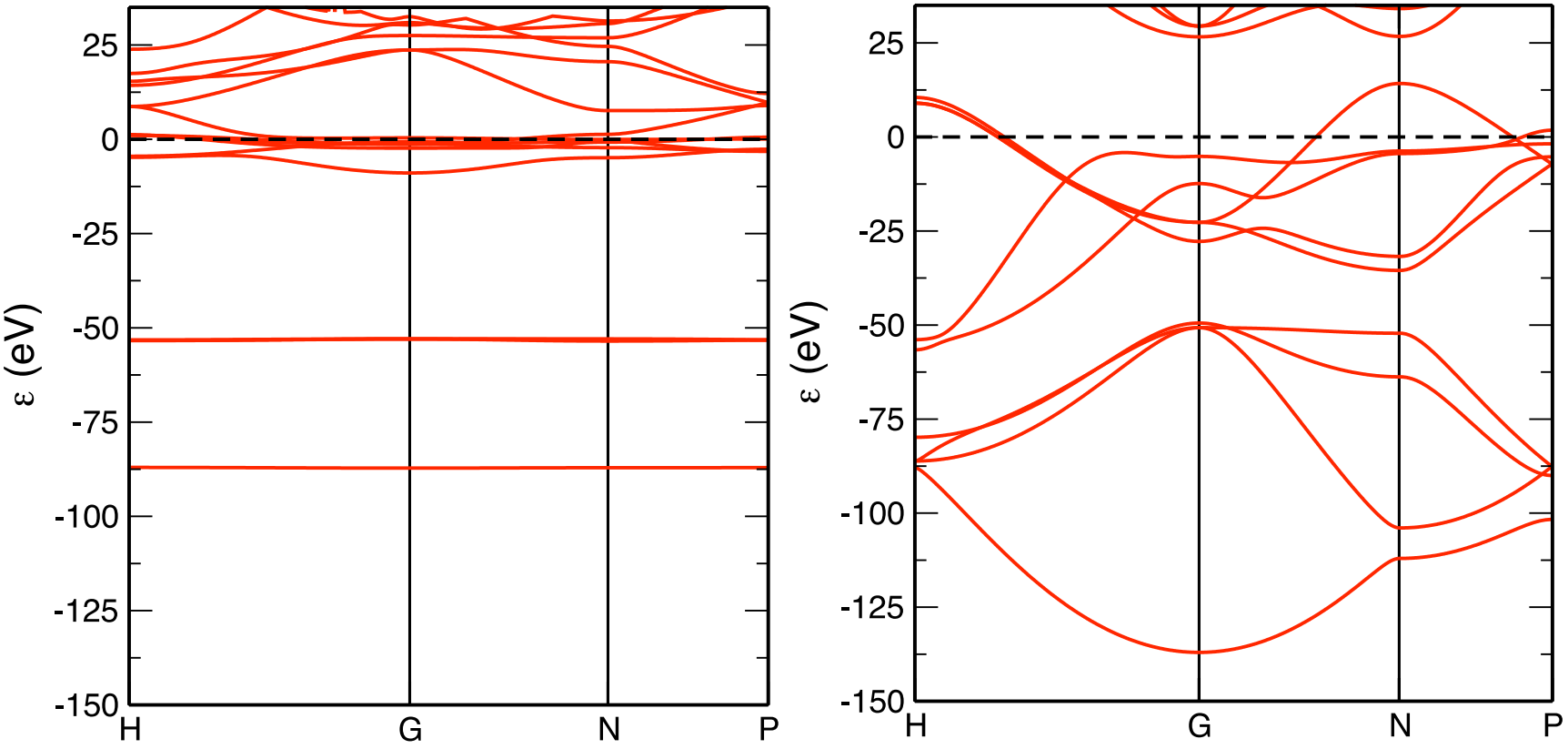
Current maximum pressure in diamond anvil cell $\simeq$ 0.35 TPa

Can achieve multi-TPa pressures in shock wave experiments

Aluminium subjected to 400 TPa in an underground nuclear explosion

Development of apparatus for multi-TPa experiments, laser driven shock waves, precompression, National Ignition Facility (NIF) etc.

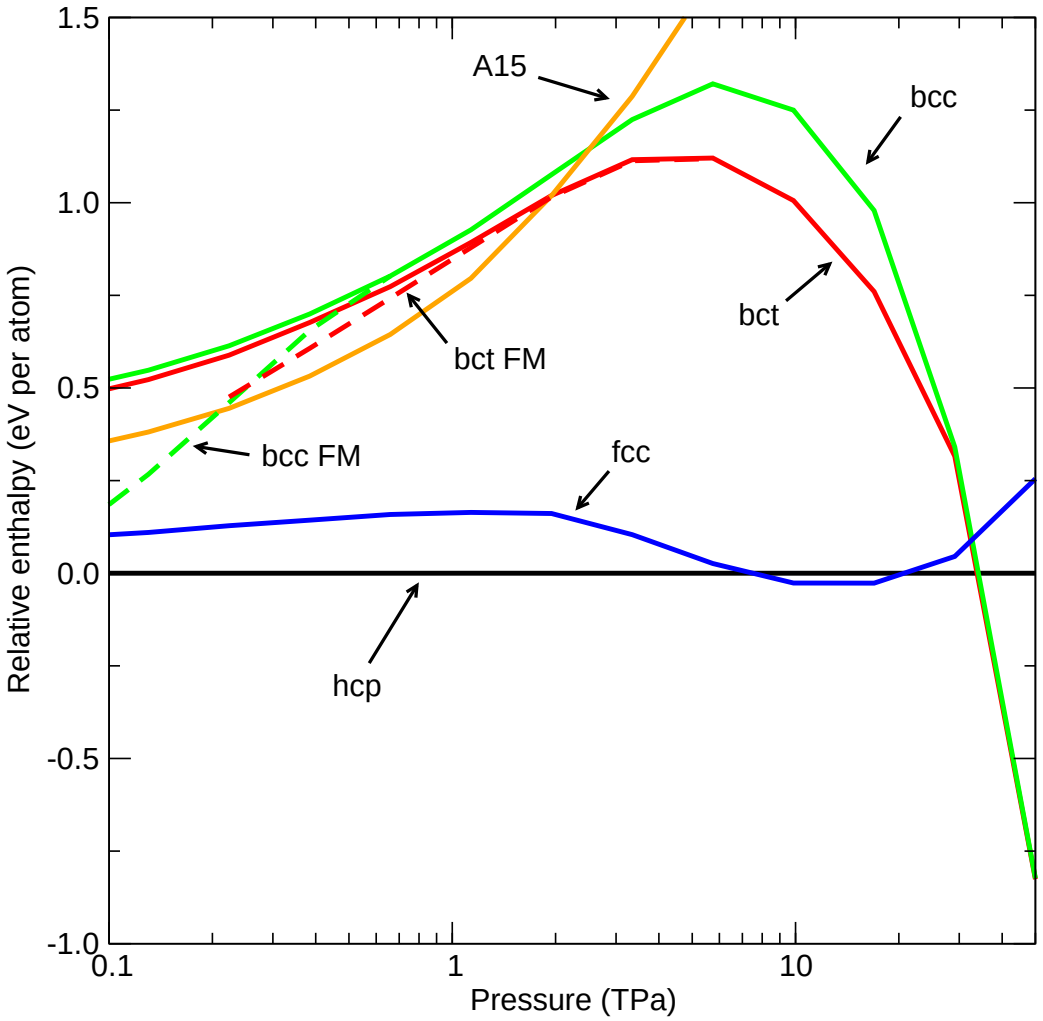
Iron at terapascal pressures



Bandstructures of (non-magnetic) bcc iron at zero pressure (left) and 30 TPa (right). The Fermi energies are at zero energy.

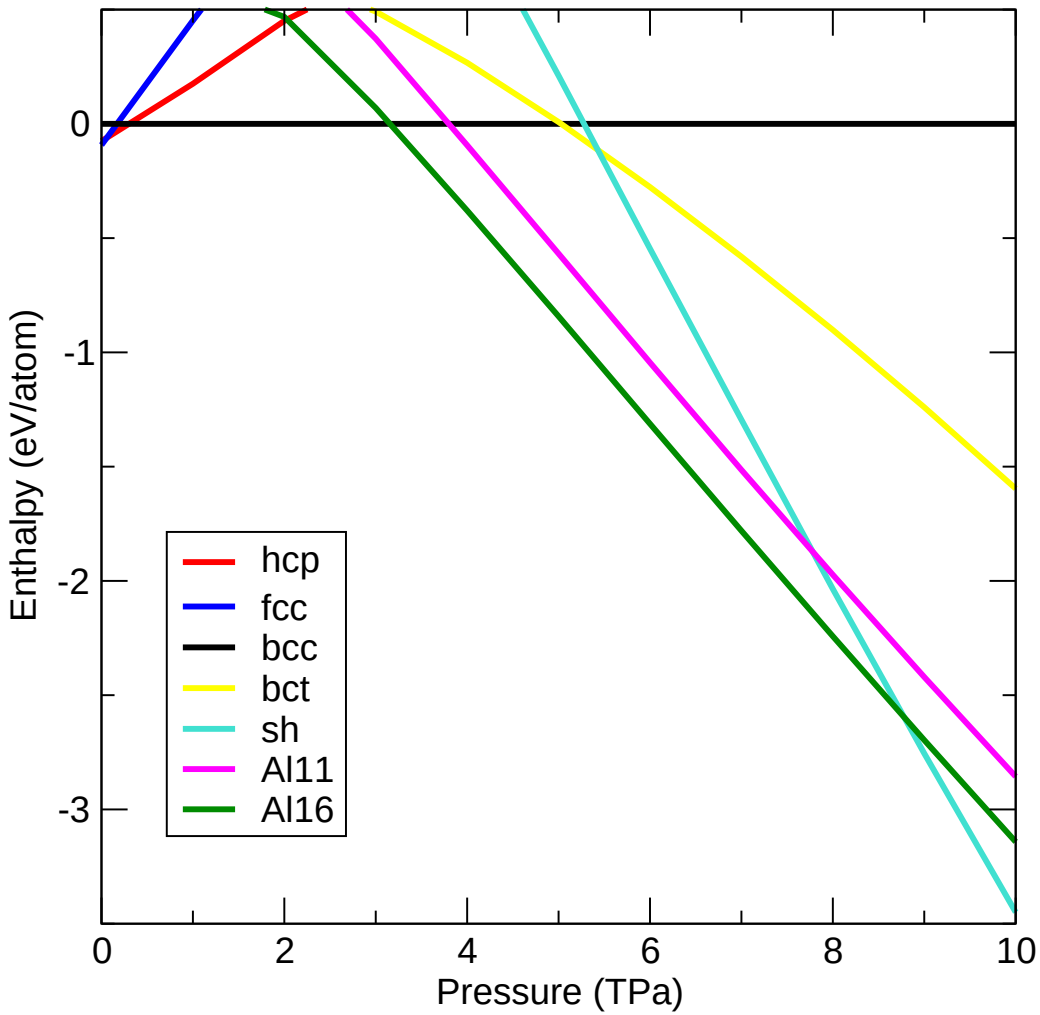
Pickard and Needs, J Phys: Condensed Matter 21, 452205 (2009)

Iron at terapascal pressures



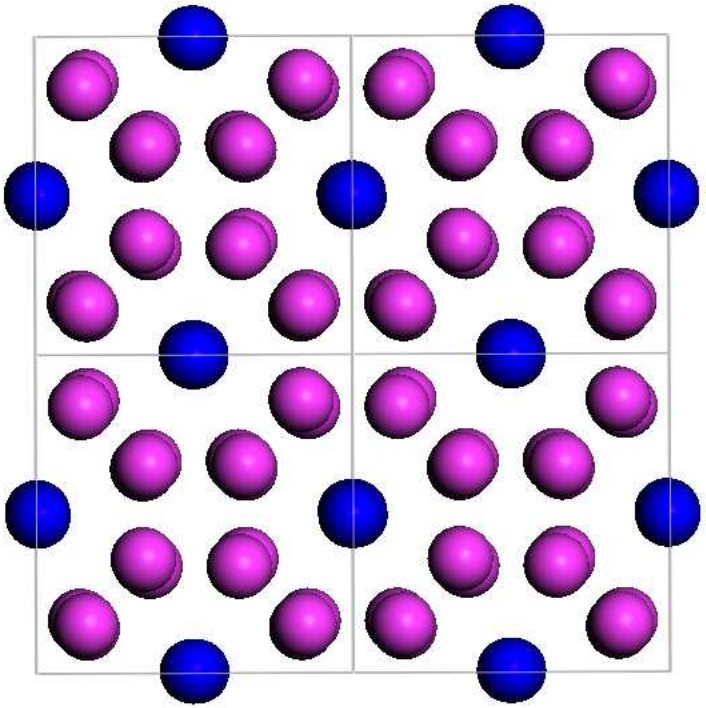
Pressure dependence of the enthalpies of various phases of iron with respect to the hcp phase. The dashed lines denote ferromagnetic (FM) phases and the solid lines denote non-magnetic phases.

Aluminium at Terapascal pressures

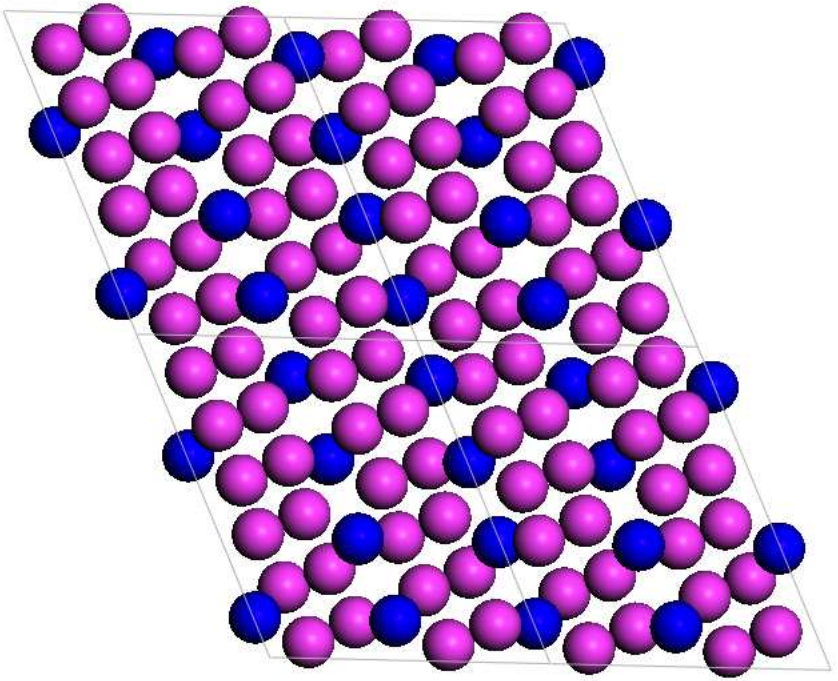


Pickard and Needs, to appear in *Nature Materials*

The Al16 structure of aluminium

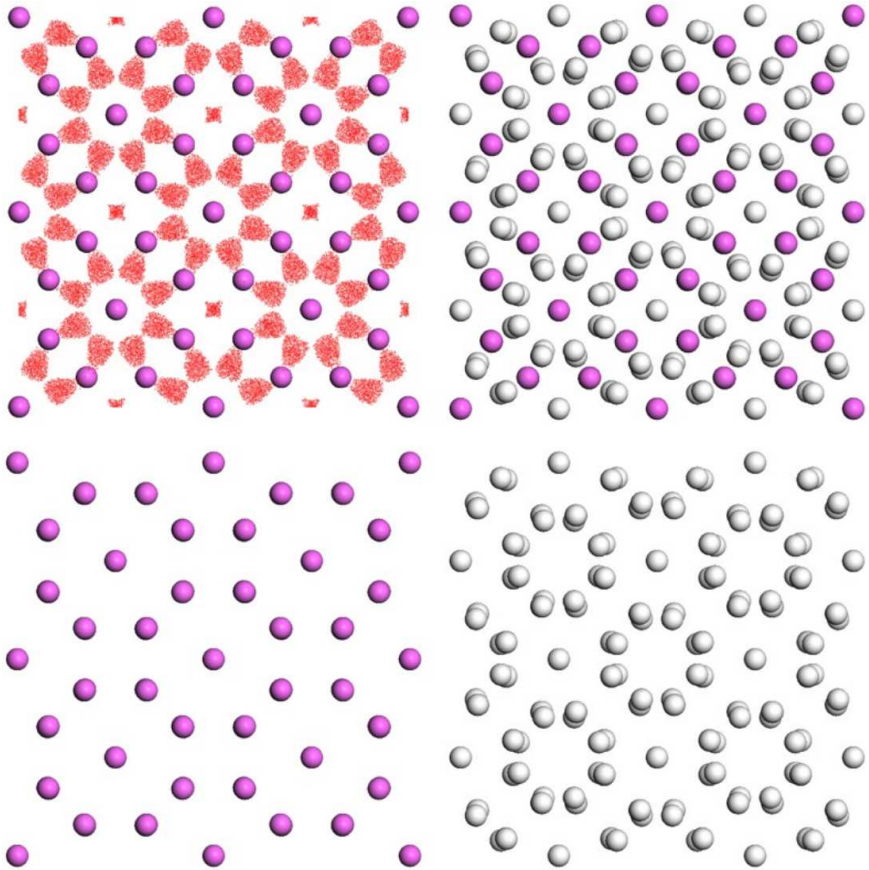


View along guest chains



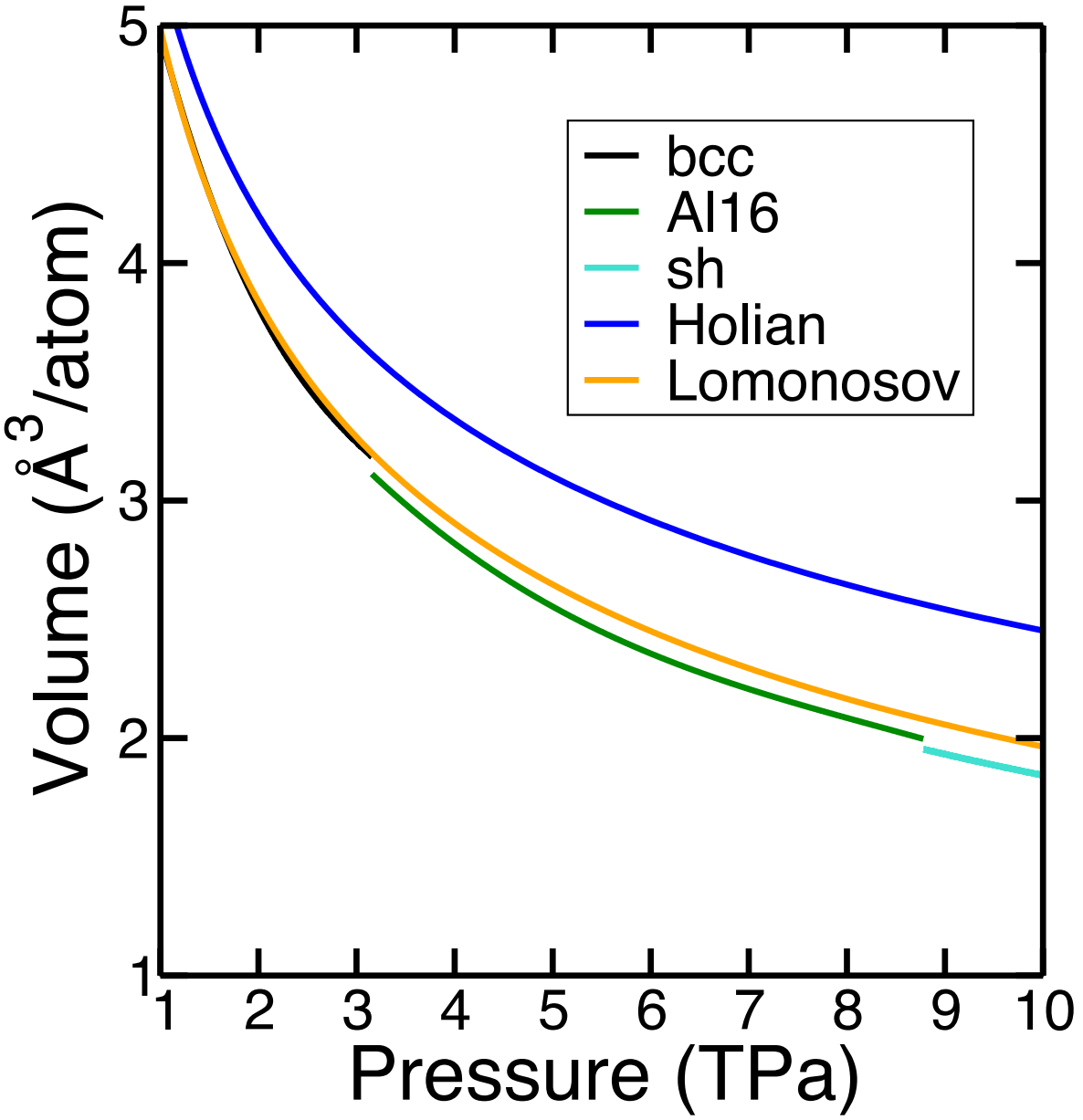
View perpendicular to chains

Incommensurate host-guest structures

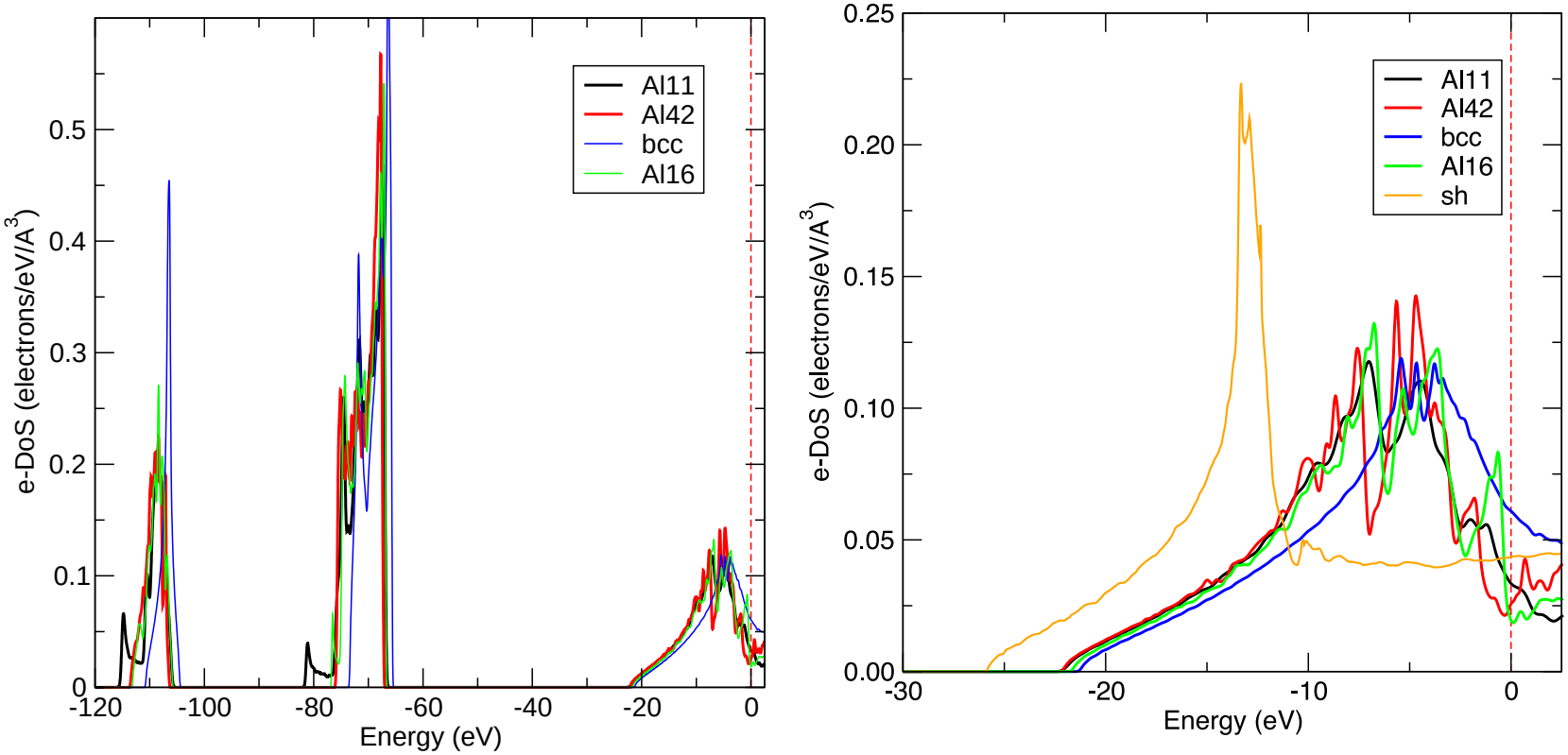


(a) Al16 host-guest structure pictured along axis of guest chains. Valence charge density >65% of maximum in red
(b) Structure from simple pairwise potentials for 16 "Al" atoms (purple) and 28 "electron" blobs (white)
(c) Purple "Al" ions from (b) give the Ba-IV structure
(d) White "electron" blobs from (b) give the Rb-IV structure

Equation of State of Aluminium

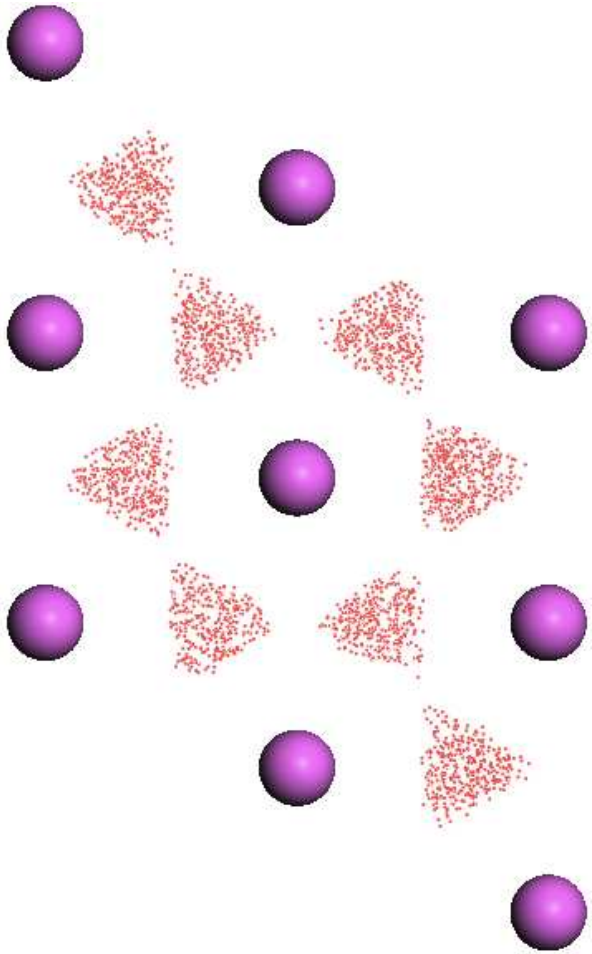


Aluminium at Terapascal pressures

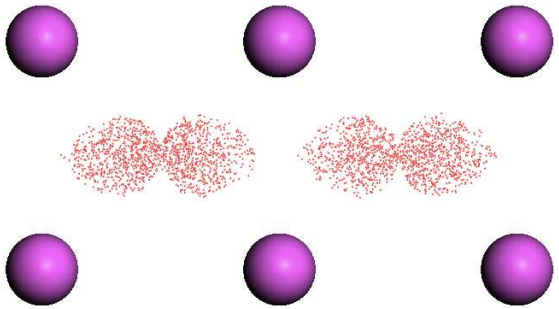


Electron densities of states

Simple Hexagonal Structure of Aluminium



Top view



Side view

Conclusions

- With care, pseudopotentials work fine at multi-TPa
- Core or semi-core states can become very important
- Iron could be bct or bcc at $p >\sim 30$ TPa (accessible to NIF)
- Aluminium forms incommensurate host-guest structure at TPa pressures, followed by strong electrides with layers of valence charge
- Electride structures are expected to be very common in highly compressed sp-bonded materials
- The return to close packing occurs at very high pressures (temperature also helps)