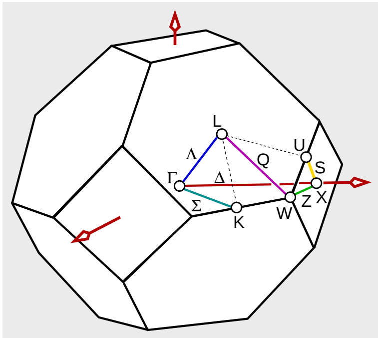
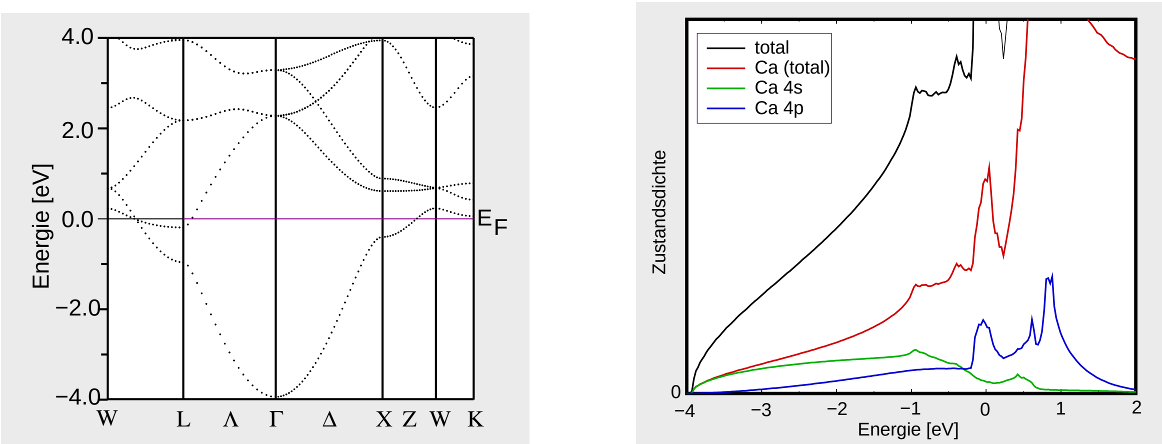
4. Bandstruktur und Bindungstyp, strukturelle Stabilitäten (Forts.)

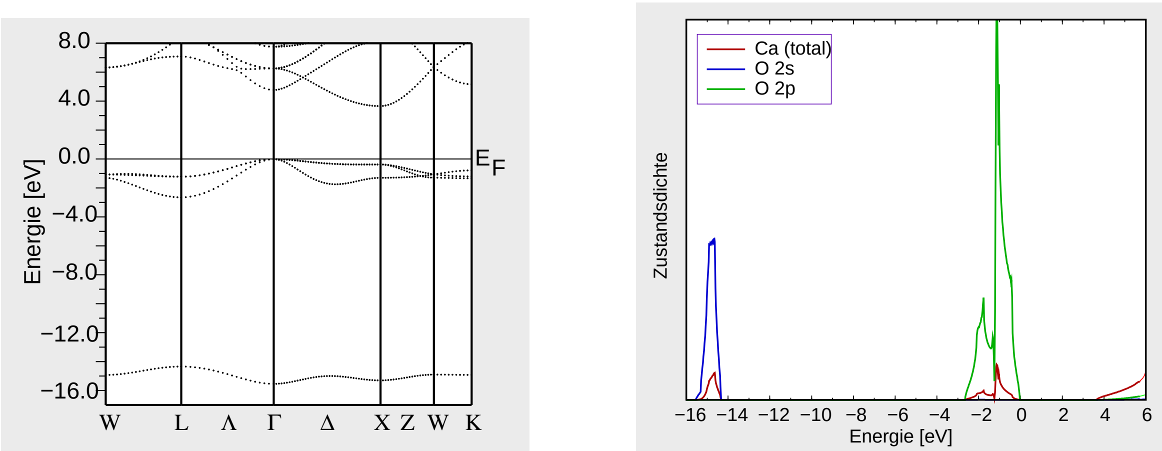
4.2. Beispiele

Berechnete Bandstrukturen/tDOS/pDOS von Strukturen mit kubischer F-Zelle:

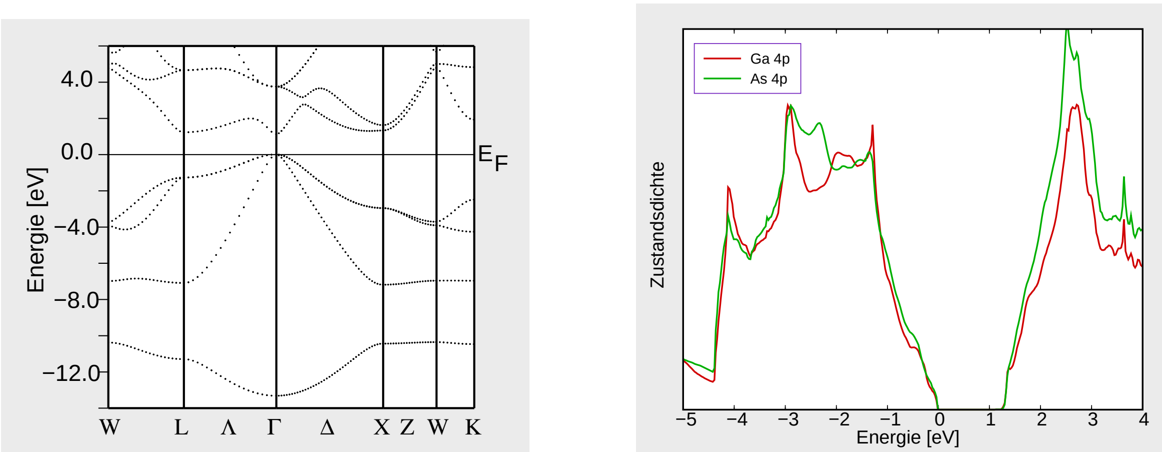




elementares Calcium (Metall)



CaO (Ionenkristall)



GaAs (kovalenter Festkörper)