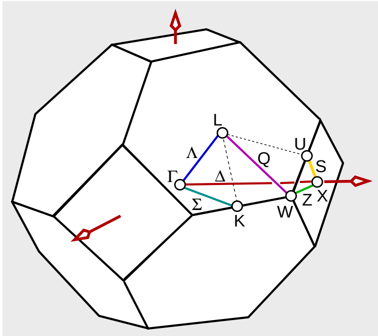
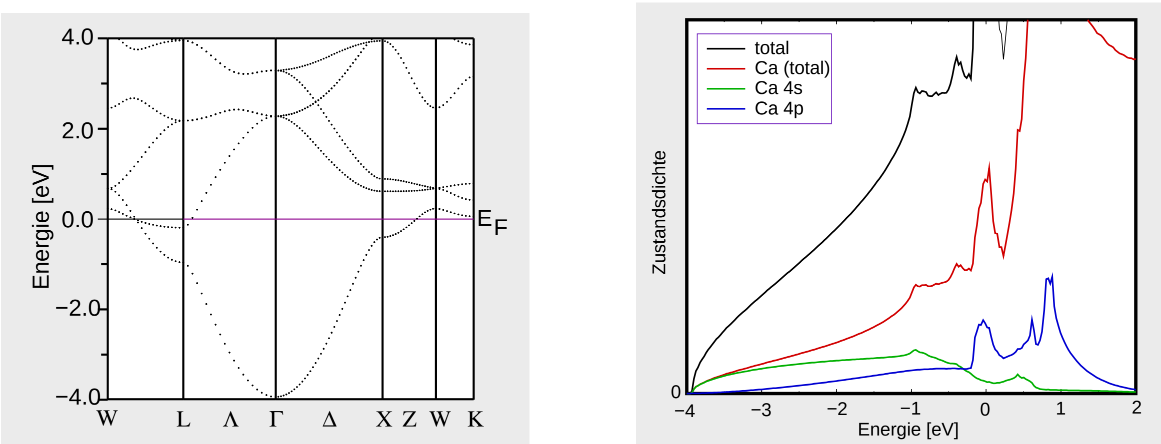
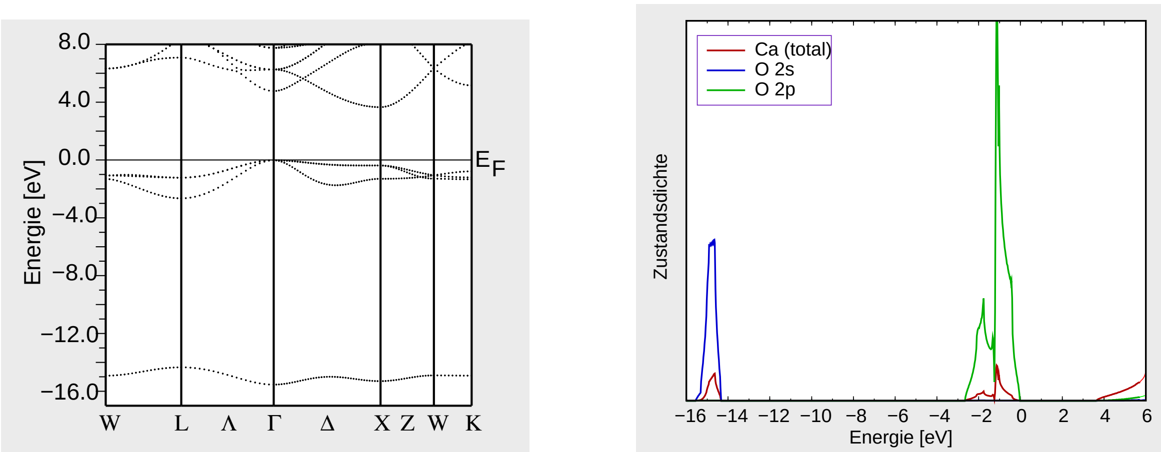
III. Berechnungen, Beispiele

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

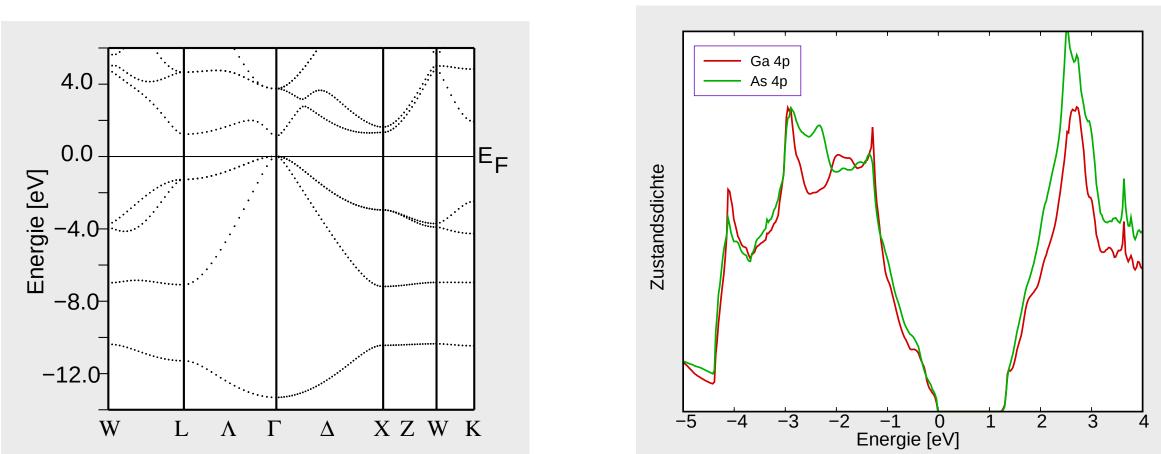




elementares Calcium (Metall)



CaO (Ionenkristall)



GaAs (kovalenter Festkörper)