

DOS and partial DOS in ABINIT: angular momentum projection and the tetrahedron method

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The traditional method for calculating the density of states has been supplemented by the tetrahedron method (TM) in ABINIT. The TM converges faster and gives better results by interpolating the band structure and calculating the resulting contribution to the DOS. Pathological cases and caveats are presented. The projection of wavefunctions on angular momenta has also been implemented, and the output (contribution of s, p, d... to each band at each kpoint) is used to output projected DOS. Implementation and user inputs are discussed.