PROJECTED DENSITY OF STATES AND MOMENTS IN TRANSITION METALS WITH SPIN DENSITY WAVES

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9.7 cm

Most calculations involving the Kohn-Sham (KS) equations such as *ab initio* molecular dynamics calculations [1], require a simplification of these equations. Our approach is based on the moment technique [2], which is an interpolation of electronic structure. The KS Hamiltonian of transition metal with spin density waves (SDW) is given in the form [3]. The KS equations, the projected density of states (PDOS), moments of PDOS and Anderson's atomic orbitals are self-consistently calculated. The moments contain the dependence of KS orbitals on the interatomic spacing and the SDW parameters, as given by the Hellmann-Feynman theorem. The moments enable us to analytically express the PDOS, the total electronic energy and the chemical potential as functions of the SDW parameters (SDW wave vector and polar angle of magnetic configuration). We use the adiabatic local density approximation. Calculations are confined to second moments of PDOS at atomic orbitals.

[1] D. Marx and J. Hutter, *Ab initio molecular dynamics: Theory and Implementation* in NIC Series, Vol. 1, John von Neumann Institute for Computing, Jülich 2000.
[2] M. J. Kelly, *Solid State Phys.* **35**, 296 (1980).
[3] M. Uhl, L.M. Sandratskii and J. Kübler *J. Magn. Magn. Mater.* **103**, 314 (1992).

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