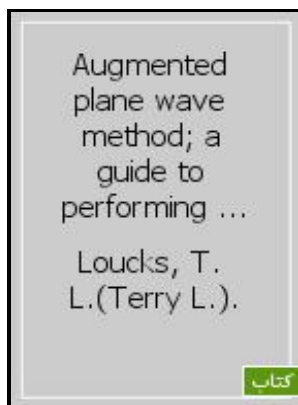


# Augmented plane wave method - a guide to performing electronic structure calculations

W.A. Benjamin - A Projector Augmented Wave (PAW) code for electronic structure calculations, Part II: pwpaw for periodic solids in a plane wave basis



Description: -

- Atomic theory. Augmented plane wave method - a guide to performing electronic structure calculations

- Frontiers in physics. Augmented plane wave method - a guide to performing electronic structure calculations

Notes: Includes bibliographies.

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ShieldSquare

The authors would like to thank Zhiqiang Mao, C. Starting from the local spin density approximation LSDA or generalised gradient approximation GGA, we verified either the orbital polarisation OP correction or the GGA + U approach for the U 5f electrons, changing Coulomb-repulsion energies U in the range 0—4 eV. A dense  $24 \times 24 \times 24$  grid was used for evaluating the accurate electron-phonon interaction matrices.

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Thermometers and the addenda were well calibrated prior to the measurements of the sample. The temperature dependence of luminescence decay kinetics provides additional evidence of the localized exciton luminescence of Bi-doped YVO 4. The electronic density of states and band structure calculations predicts the metallic behavior of the compounds in GGA, whereas, by the GGA + U approach, half-metallic ferromagnetism HMF is predicted.

**A Projector Augmented Wave (PAW) code for electronic structure calculations, Part II: pwpaw for periodic solids in a plane wave basis**

The formalism of calculating the ortho-elastic constants is described in details.

**Phys. Rev. B 82, 155121 (2010)**

The full-potential linearized augmented plane waves method was used with the generalized gradient approximation for the exchange-correlation potential with Perdew, Burke and Ernzerhof functional.

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