We discuss abilities of the exact Fock exchange \( \mathcal{E}_X \) to deal with the phenomenon of the orbital magnetism in density functional theory. The essence of our approach is to decompose the density matrix in terms of invariant \((\mathbf{R}_k, \mathbf{p})\) and noninvariant \((\mathbf{R}_k, \mathbf{p})\) parts under the time reversal operation. By stressing the short-range electron-electron interactions, we analyze the exchange enhancement of the orbital magnetisation given by \( \mathcal{E}_X \). For \( \mathcal{E}_X \) it leads to Stoner-like orbital exchange \( \mathcal{E}_X[t] = \{ -1 \} \sum I \mathcal{E}_X(t) \} \) driven by on-site Coulomb interaction \( \mathcal{U} \). More generally, \( \mathcal{E}_X \) can be expressed in terms of expectation values of the irreducible set of operators being odd order products of \( I \) and \( \mathcal{L} \). Local enhancement of the crystal field effects in \( \mathcal{E}_X \) as well as Hartree term \( \mathcal{E}_H \) relevant to the quenching of the orbital moments is driven by the same parameter \( (\mathcal{U}) \) and should be considered on an equal footing with \( \mathcal{E}_X \). We have implemented this formalism in the spirit of rotationally invariant LDA+U approach\(^{(1)}\) in the fully relativistic LMTO method. Applications for Fe, Co and Ni as well as equilibrium magnetic ordering in FeO and CoO will be given. The work is partly supported by NEDO.

References


29a-P-2

\( \text{Cr}^2+ \) and \( \text{Ce}^4 \)の弹性異常と結晶場効果

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Hyperspectral Raman scattering and related experiments show that the anharmonic process in \( \text{Cr}^2+ \) is enhanced by the \( \text{Ce}^4 \) fluctuation, which is responsible for the observed anomaly in the elastic constants.

29a-P-3

Efficient Calculation of Exchange Energy in the Local Spin Density Approximation

Y. Tanaka, M. Ikeda, H. Fujimoto, H. Watanabe, T. Sato

We present an efficient and accurate algorithm for the calculation of the exchange energy in the local spin density approximation, which is a key component in density functional theory. The algorithm is based on a novel representation of the exchange potential, and it has been implemented in a practical computational code. The results show excellent agreement with benchmark data.

29a-P-4

Spin-Polarized Band Structure Calculations

J. P. Perdew, K. Burke, M. Ernzerhof

We present a new functional for density functional theory that is specifically designed to accurately describe correlated systems such as magnetism. The functional is based on a novel ansatz for the exchange-correlation energy that is inspired by the physics of the spin-polarized band structure. We demonstrate the efficacy of the functional using a series of benchmark calculations.

29a-P-5

Orbital Magnetism in Band Structure Calculations

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We discuss abilities of the exact Fock exchange \( \mathcal{E}_X \) to deal with the phenomenon of the orbital magnetism in density functional theory. The essence of our approach is to decompose the density matrix in terms of invariant \((\mathbf{R}_k, \mathbf{p})\) and noninvariant \((\mathbf{R}_k, \mathbf{p})\) parts under the time reversal operation. By stressing the short-range electron-electron interactions, we analyze the exchange enhancement of the orbital magnetisation given by \( \mathcal{E}_X \). For \( \mathcal{E}_X \) it leads to Stoner-like orbital exchange \( \mathcal{E}_X[t] = \{ -1 \} \sum I \mathcal{E}_X(t) \} \) driven by on-site Coulomb interaction \( \mathcal{U} \). More generally, \( \mathcal{E}_X \) can be expressed in terms of expectation values of the irreducible set of operators being odd order products of \( I \) and \( \mathcal{L} \). Local enhancement of the crystal field effects in \( \mathcal{E}_X \) as well as Hartree term \( \mathcal{E}_H \) relevant to the quenching of the orbital moments is driven by the same parameter \( (\mathcal{U}) \) and should be considered on an equal footing with \( \mathcal{E}_X \). We have implemented this formalism in the spirit of rotationally invariant LDA+U approach\(^{(1)}\) in the fully relativistic LMTO method. Applications for Fe, Co and Ni as well as equilibrium magnetic ordering in FeO and CoO will be given. The work is partly supported by NEDO.

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