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Density Functional Theory and Noncollinear Magnetism JUAN PERALTA, Department of Chemistry, Rice University, Houston, Texas — We present a generalization of the treatment of the electronic spin degrees of freedom in density functional calculations to the case where the spin can vary in any direction in space. This generalization is applied not only to the local–spin density and generalized–gradient approximations, but also to meta–generalized gradient energy functionals that include the kinetic energy density and the Laplacian of the density in their ingredients, as well as to hybrid functionals including Hartree–Fock exchange. The expression of the generalized exchange and correlation potential matrix elements is explicitly derived for all cases. We discuss the model case of planar Cr clusters that exhibit ground states with noncollinear spin densities due to geometrically frustrated antiferomagnetic interactions.

Juan E. Peralta
Department of Chemistry, Rice University, Houston, Texas

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