

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Construction of an analytic exchange-correlation hole for the Perdew-Burke-Ernzerhof GGA MATTHIAS ERNZERHOF, Department of Chemistry, University of Montreal, HILKE BAHMANN, Department of Chemistry, University of Wuerzburg — The Perdew-Burke-Ernzerhof (PBE) [1] approximation to the exchange-correlation energy is employed as a starting point for the construction of an approximate, spherically averaged exchange-correlation hole. In a first step, we develop a new model for the PBE exchange hole. This model satisfies the homogeneous electron gas limit; it is normalized and yields the correct small-gradient limit in the system average. A correlation factor [2], i.e., a function multiplying the exchange hole, is proposed that turns the exchange into an exchange-correlation hole. The correlation factor has a simple form and its parameters are determined through a number of known conditions that ought to be satisfied by a PBE exchange-correlation hole. The homogeneous-electron-gas limit of the new hole model is compared to the LSD hole [3].

[1] J.P. Perdew, K. Burke, M. Ernzerhof, PRL 77, 3865 (1996); 78, 1396(E) (1997).

[2] P. Gori-Giorgi, J.P. Perdew, PRB 66, 165118 (2002).

[3] J.P. Perdew, Y. Wang, PRB 46, 12947 (1992).

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Date submitted: 29 Nov 2007

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