Functional: Perdew & Wang
Type: LDA
XC: Correlation
References:

- J.P. Perdew and Y. Wang, Phys. Rev. B **45**, 13244 (1992) APS
- Ortiz and Ballone, Phys. Rev. B **50**, 1391 (1994) APS
- Ortiz and Ballone, Phys. Rev. B **56**, 9970(E) (1997) APS

For finite spin-polarization , Perdew and Wang parametrized the correlation energy per unit particle in the following way:

$$e_c(r_s,\zeta) = e_c(r_s,0) + \alpha_c(r_s)\frac{f(\zeta)}{f''(0)}(1-\zeta^4) + [e_c(r_s,1) - e_c(r_s,0)]f(\zeta)\zeta^4$$

The function *f*( ) is

$$f(\zeta) = \frac{[1+\zeta]^{4/3} + [1-\zeta]^{4/3} - 2}{2^{4/3} - 2},$$

while its second derivative *f*''(0) = 1.709921

The three functions, $e_c(r_s,0)$ (the paramagnetic energy of the e-gas), $e_c(r_s,1)$ (the ferromagnetic energy of the e-gas), and – $_c(r_s)$ (note the minus sign) are all parametrized by the function

$$g = -2A(1+\alpha_1 r_s)\log\left\{1 + \frac{1}{2A(\beta_1 r_s^{1/2} + \beta_2 r_s + \beta_3 r_s^{3/2} + \beta_4 r_s^2)}\right\}$$

There are two parametrizations using this form, the original from Perdew and Wang, and a later version by Ortiz and Ballone. The coefficients are the following

	Perdew & Wang			Ortiz & Ballone		
	$e_c(r_s,0)$	$e_c(r_s,1)$	– (r_s)	$e_c(r_s,0)$	$e_c(r_s,1)$	– (r_s)
A	0.031091	0.015545	0.016887	0.031091	0.015545	0.016887
$_1$	0.21370	0.20548	0.11125	0.026481	0.022465	0.11125
$_1$	7.5957	14.1189	10.357	7.5957	14.1189	10.357
$_2$	3.5876	6.1977	3.6231	3.5876	6.1977	3.6231
$_3$	1.6382	3.3662	0.88026	-0.46647	-0.56043	0.88026
$_4$	0.49294	0.62517	0.49671	0.13354	0.11313	0.49671