

```
[13] from pylibxc import LibXCFunctional
import pylibxc.util
print(pylibxc.util.xc_version())
print(pylibxc.util.xc_version_string())
print(pylibxc.util.xc_number_of_functionals())
```

(4, 2, 3)

4.2.3

446

```
[22] for id in pylibxc.util.xc_available_functional_numbers():
      name = pylibxc.util.xc_functional_get_name(id)
      if 'pbe' in name:
          print(id, name)
```

49 gga_x_pbe_mol
53 gga_k_revapbeint
54 gga_k_apbeint
55 gga_k_revapbe
59 gga_x_pbe_tca
60 gga_x_pbeint
61 gga_c_zpbeint
62 gga_c_pbeint
63 gga_c_zpbesol
65 gga_xc_opbe_d
69 gga_x_vmt84_pbe
71 gga_x_vmt_pbe
86 gga_c_op_pbe
89 gga_c_spbe
101 gga_x_pbe
102 gga_x_pbe_r
116 gga_x_pbe_sol
117 gga_x_rpbe
121 gga_x_pbea
122 gga_x_mpbe
123 gga_x_xpbe
126 gga_x_pbe_jsjr
129 gga_x_2d_pbe
130 gga_c_pbe
133 gga_c_pbe_sol
136 gga_c_xpbe
138 gga_c_pbe_jrgx
140 gga_x_pbek1_vdw
141 gga_x_optpbe_vdw
173 gga_xc_pbe1w
175 gga_xc_pbelyp1w
184 gga_x_apbe
185 gga_k_apbe

186 gga_c_apbe
246 gga_c_pbeloc
258 gga_c_pbefe
265 gga_x_pbefe
272 gga_c_pbe_mol
291 gga_x_pbetrans
524 gga_x_wpbeh
525 gga_x_hjs_pbe
526 gga_x_hjs_pbe_sol
539 gga_x_pbepow
557 gga_c_zvpbeint
558 gga_c_zvpbesol
560 gga_c_tm_pbe
595 gga_k_pbe3
596 gga_k_pbe4
273 hyb_gga_xc_pbe_mol0
274 hyb_gga_xc_pbe_sol0
275 hyb_gga_xc_pbeb0
276 hyb_gga_xc_pbe_molb0
290 hyb_gga_xc_pbe50
406 hyb_gga_xc_pbeh
429 hyb_gga_xc_hjs_pbe
430 hyb_gga_xc_hjs_pbe_sol
456 hyb_gga_xc_pbe0_13
465 hyb_gga_xc_lrc_wpbeh
467 hyb_gga_xc_lcy_pbe
472 hyb_gga_xc_hpbeint
473 hyb_gga_xc_lrc_wpbe
478 hyb_gga_xc_lc_wpbe
484 hyb_gga_xc_mpwlpbe
576 mgga_x_pbe_gx
568 hyb_mgga_xc_pbe1kcis

```
[20] lda_x = LibXCFunctional('LDA_X', spin=1)
      print(lda_x.describe())
```

Functional ID: 1

Functional Name: lda_x

Attributes:

 Name: Slater exchange

 Kind: 0

 Family: 1

Citations:

 P. A. M. Dirac, Math. Proc. Cambridge Philos. Soc. 26, 376 (1930)

 F. Bloch, Z. Phys. 57, 545 (1929)

```
[21] lda_c_pz = LibXCFunctional('LDA_C_PZ', spin=1)
      print(lda_c_pz.describe())
```

Functional ID: 9

Functional Name: lda_c_pz

Attributes:

Name: Perdew & Zunger

Kind: 1

Family: 1

Citations:

J. P. Perdew and A. Zunger, Phys. Rev. B 23, 5048 (1981)

```
[26] test = LibXCFunctional(65, spin=1)
      print(test.describe())
```

Functional ID: 65

Functional Name: gga_xc_opbe_d

Attributes:

Name: oPBE-D functional of Goerigk and Grimme

Kind: 2

Family: 2

Citations:

L. Goerigk and S. Grimme, J. Chem. Theory Comput. 6, 107 (2010)

```
[31] print(LibXCFunctional('gga_x_pbe_sol', spin=1).describe())
      print()
      print(LibXCFunctional('gga_c_pbe_sol', spin=1).describe())
```

Functional ID: 116

Functional Name: gga_x_pbe_sol

Attributes:

Name: Perdew, Burke & Ernzerhof SOL

Kind: 0

Family: 2

Citations:

J. P. Perdew, A. Ruzsinszky, G. I. Csonka, O. A. Vydrov, G. E. Scuseria, L. A. Constantin, X. Zhou, and K. Burke, Phys. Rev. Lett. 100, 136406 (2008)

Functional ID: 133

Functional Name: gga_c_pbe_sol

Attributes:

Name: Perdew, Burke & Ernzerhof SOL

Kind: 1

Family: 2

Citations:

J. P. Perdew, A. Ruzsinszky, G. I. Csonka, O. A. Vydrov, G. E. Scuseria, L. A. Constantin, X. Zhou, and K. Burke, Phys. Rev. Lett. 100, 136406 (2008)

