New Density Functionals

- DFT is the most successful method for the calculation of the electronic structure, properties, and potential energy surfaces of all but the smallest chemical systems.
- The development of improved approximations to the exchange-correlation functional has been a crucial ingredient in the success of DFT
- The optimization of new functionals depends on two factors:
  - the functional form must be physically appropriate and flexible enough to catch most of the possible systematic improvements, but not too flexible, in order to avoid over-fitting.
  - the databases used in the process must include a large number of data for different properties, avoiding however data that is beyond the predictive ability of the chosen functional form.

We introduced a new generation of approximation to the exchange-correlation functional called the 11 Generation.

There are four new functionals in the set:

SOGGA11
SOGGA11-X

M11-L M11

The M11 functionals are the most accurate.

The SOGGA11 functionals are best in their class for simpler functional forms.

Peverati, Zhao, Truhlar (Univ. of Minnesota)

Second-Order GGA family

SOGGA11

- The first GGA correct to second order that provide good accuracy for a broad variety of chemical problems.
- Simple implementation in any quantum chemistry software

SOGGA11-X

- The most successful hybrid-GGA for chemical calculation of a broad variety of chemical problems.
- Simple implementation in any quantum chemistry software

Performance of SOGGA11 compared to other GGA functionals for a broad chemistry database:

Functional	MUE (kcal/mol)	Functional	MUE (kcal/mol)
PBE	7.27	HCTH407	4.47
BP86	6.56	RPBE	4.46
BLYP	5.16	BPW91	4.32
revPBE	4.74	OLYP	4.19
mPWPW	4.62	**SOGGA11**	**3.77**

Performance of SOGGA11-X compared to other hybrid GGA functionals for a broad chemistry database:

Functional	MUE (kcal/mol)	Functional	MUE (kcal/mol)
PBE0	4.86	O3LYP	3.02
B1LYP	3.90	B3PW91	2.99
B3LYP	3.67	B98	2.81
mPW1PW	3.13	B97-3	2.43
		SOGGA11-X	**1.93**

MUE is mean unsigned error.

SOGGA11: Peverati, Zhao, Truhlar; J.Phys Chem. Lett. 2, 1991(2011) [2]
SOGGA11-X: Peverati, Truhlar; J. Chem. Phys. 135, in press

Minnesota 11 meta-GGA family

M11

- The first range-separated hybrid meta-GGA optimized for a broad variety of chemical problems.
- Big improvement over the previous generation of very successful Minnesota functionals (M05, M06, and M08)

M11-L

- The first dual-range local meta-GGA functional.
- The first local functional to have similar accuracy as hybrid functionals, but local has a much lower computational cost.
- Good performances for chemistry and solid-state physics calculations.

Performance of M11 and M11-L compared to other Minnesota meta-GGA functionals for a broad chemistry database:

Functional:	M05	M05-2X	M06-L	M06	M06-2X	M06-HF	**M11-L**	**M11**
MUE: (kcal/mol)	2.88	2.31	3.24 (local)	2.30	2.11	3.17	**2.52** (local)	**1.84**

M11: Peverati, Truhlar; J.Phys Chem. Lett. 2, 2810 (2011)
M11-L: Peverati, Truhlar; manuscript in preparation.