

## Assessment of a New Hybrid Functional on Thermochemistry, Metal-Ligand Bonding and Reaction Barriers

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### Abstract

The meta-GGA correlation functional tLap proposed recently is used to develop a new hybrid combination, B3tLap. Validation tests in comparison with some current top notch functionals are discussed. The new functional is on average slightly better than B3LYP, BMK and M06 for atomization energies and metal-ligand bonding, while using less fitting parameters. For difficult reaction barriers B3tLap is slightly inferior to M06 and BMK, but more accurate than B3LYP.

### Nomenclature

|                          |   |   |
|--------------------------|---|---|
| $E_{x\sigma}$            | = | $\sigma$ - $\sigma$ spin component of the exchange energy                           |
| $E_c^{\sigma\sigma'}$    | = | $\sigma$ - $\sigma'$ spin-spin component of the correlation energy                  |
| $E_{xc}$                 | = | total (spin-summed) exchange-correlation energy                                     |
| $t_{s\sigma}$            | = | $\sigma$ -spin component of the kinetic energy density including the Laplacian term |
| $\tau_\sigma$            | = | $\sigma$ -spin component of the kinetic energy density without the Laplacian term   |
| $k_\sigma$               | = | parallel-spin (in $\sigma$ direction) correlation wave vector                       |
| $k_{\uparrow\downarrow}$ | = | opposite-spin correlation wave vector   |
| $D_e$                    | = | atomization energy without the zero-point vibrational contribution                  |

### 1 Introduction

Finding new accurate exchange-correlation (XC) functionals is a paramount in density functional theory (DFT). In a conference talk in 1992 Becke justified the combination of the Generalized Gradient Approximation (GGA) and the Hartree-Fock (HF) exchange in a single exchange-correlation scheme. This idea was further developed to create the class of hybrid functionals [1]. Various realizations of the hybrid scheme were proposed later on based on different GGA and meta-GGA components. The latter involve the kinetic-energy density as a non local variable that is highly sensitive to effects of inhomogeneity. The hybrid functional B3LYP [1,2] is one of the most used to date. The PBE0 and TPSS functionals [3] are non empirical realizations of the hybrid approach, sometimes

more accurate than B3LYP, sometimes not. The M0 series of multi-parameter functionals (M05, M06, M062X) [4,5] are perhaps one of the most accurate to date for many, but not for all systems. Concerning catalytic studies, it is desirable to have a functional that performs uniformly well for atoms, small and large molecules and solid systems. This is particularly important in studying adsorption processes and surface reactions, since a non uniform performance of a given method would lead to less accurate energy differences in such cases. In this work we suggest a new hybrid functional that has less empirical parameters than most of the other hybrid versions, while having on average better accuracy. The model is based on the recent tLap meta-GGA correlation functional [6]. One should note that a functional from the Lap series [6,7] has not been tested yet in a hybrid combination. Validation tests in comparison with some current top notch functionals are discussed.

## 2 Theoretical Gist

In KS DFT the exchange-correlation energy is usually cast in a hydrodynamic-like form in terms of separate spin-spin components:

$$E_{xc}[n_{\uparrow}, n_{\downarrow}] = \int d\mathbf{r} n(\mathbf{r}) \varepsilon_{xc}(\mathbf{r}), \quad n = n_{\uparrow} + n_{\downarrow}, \quad (1)$$

$$\varepsilon_{xc}(n_{\uparrow}, n_{\downarrow}) = \sum_{\sigma} \varepsilon_{x\sigma}(n_{\sigma}) + \sum_{\sigma} \varepsilon_c^{\sigma\sigma}(n_{\sigma}) + \varepsilon_c^{\uparrow\downarrow}(n_{\uparrow}, n_{\downarrow}) \equiv \varepsilon_x + \varepsilon_c. \quad (2)$$

Various methods of functional development have been advanced over the years. The meta-GGA correlation functional tLap used in this work was derived in the context of the adiabatic connection method using model pair correlation functions with a correct cusp [6]. It presents an improvement over the Lap3 and  $\tau_1$  functionals derived earlier following a similar approach [7,8]. All these have a compact analytic form involving only the electron density and the so called correlation wave vectors  $k_{\sigma\sigma'}$  [6]. The tLap functional employed here reads:

$$\varepsilon_c^{\uparrow\downarrow} = \frac{n_{\uparrow}n_{\downarrow}}{n} Q(k_{\uparrow\downarrow}), \quad n = n_{\uparrow} + n_{\downarrow}, \quad (3)$$

$$\varepsilon_c^{\sigma\sigma} = \frac{1}{2} \left(1 - \frac{1}{N_{\sigma}}\right) \frac{n_{\sigma}^2}{n} Q(k_{\sigma\sigma}), \quad (4)$$

$$Q(k) = -\frac{b_1}{1+b_2k} + \frac{b_3}{k} \ln\left(\frac{b_4+k}{k}\right) + \frac{b_5}{k} - \frac{b_6}{k^2}, \quad (5)$$

where  $b_i$  are coefficients yielded by the algebra [6,7],  $N_{\sigma}$  is the total number of electrons with spin  $\sigma$  entering a Fermi-Amaldi type self-interaction correction (SIC) factor [7]. The form of the wave vectors  $k_{\sigma\sigma'}$  has to be specified additionally and enters as an input to this expression. Various different functional forms can in fact be generated from Eqs. (3–5) depending on the form of  $k_{\sigma\sigma'}$  used [6,9]. A more elaborated form of the correlation wave vectors was obtained in [6] based on uniform electron gas tests and the so called similarity hypothesis: even though the uniform electron gas is rather different from a real finite

system, some similarity seems to exist in the way electron correlation changes when passing from regions of high electron density to regions of low density. The final form of the correlation wave vectors used in the tLap functional and in this work reads [6]

$$k_{\sigma\sigma}^2 = \alpha_e^2 \alpha_{\text{eff}}^2(n) \frac{10}{3} \frac{t_{s\sigma}}{n_\sigma}, \quad (6)$$

$$k_{\uparrow\downarrow}(\mathbf{r}) = \beta_e \beta_{\text{eff}}(n) \frac{2b_{s\uparrow}b_{s\downarrow}}{\left(\sqrt{n_\uparrow}b_{s\downarrow} + \sqrt{n_\downarrow}b_{s\uparrow}\right)}, \quad b_{s\sigma} = \sqrt{\frac{10}{3}t_{s\sigma}}, \quad (7)$$

where  $t_{s\sigma}$  is the electron kinetic energy density in its ‘Laplacian’ definition:

$$t_{s\sigma} = \tau_\sigma - \frac{1}{8} \nabla^2 n_\sigma, \quad \tau_\sigma = \frac{1}{2} \sum_i |\nabla \varphi_{i\sigma}|^2, \quad (8)$$

$\varphi_{i\sigma}$  are the occupied KS spin-orbitals. All non-local variables here are embodied in the correlation wave vectors and thus enter the functional in a highly non linear fashion. A special role play the two scaling parameters  $\alpha_e$  and  $\beta_e$ , which are the only two fitting parameters in tLap, and the screening functions  $\alpha_{\text{eff}}(n)$  and  $\beta_{\text{eff}}(n)$ . The latter are derived in [6,9] based on an interpolation to a precise uniform electron gas benchmarks. The tLap correlation functional was optimized in conjunction with the GGA exchange of Becke (88) [10] to form the (non hybrid) combination BtLap [6]. In this work we report for the first time results with the hybrid extension of BtLap, named here ‘B3tLap’. After the parameter optimization based on the Lap test set [6], the B3tLap hybrid scheme reads:

$$E_{xc}^{\text{B3tLap}} = 0.1713E_x^{\text{HF}} + 0.726E_x^{\text{B88}} + 0.0966E_x^{\text{LSD}} + E_c^{\text{tLap}} \quad (9)$$

In contrast to the popular B3LYP, we do not include any LSD correlation in the mixture, while a small fraction of LSD exchange is retained here. This fraction seems important to have when the Becke 88 GGA is involved in a hybrid combination. The exact-exchange fraction here is slightly smaller than what is customary used in hybrids based on GGA components only (B3LYP, PBE0). The two parameters in the tLap correlation component have the following optimized values here:  $\alpha_e = 2.515$ ,  $\beta_e = 1.085$ . These are only slightly different from the values used in the ‘pure-DFT’ combination BtLap [6]:  $\alpha_e = 2.53$ ,  $\beta_e = 1.087$ . The B3tLap hybrid functional was implemented self-consistently in the Q-Chem code [11]. In MO-LCGTO representation, the matrix elements of the XC potential ( $V_{\mu\nu}^{xc,\sigma}$ ) are determined by differentiating the XC energy matrix over the density matrix ( $P_{\mu\nu}^\sigma$ ) [6]:

$$V_{\mu\nu}^{xc,\sigma} = \frac{\partial E_{xc}}{\partial P_{\mu\nu}^\sigma} = \sum_i \frac{\partial f_{xc}}{\partial g_i} \frac{\partial g_i}{\partial P_{\mu\nu}^\sigma}, \quad (10)$$

where  $f_{xc}$  is the exchange-correlation kernel being a function of the functional variables  $g_i$ :

$$E_{xc} = \int f_{xc}(g_1, g_2, \dots, g_i, \dots) d\mathbf{r}. \quad (11)$$

In this way we avoid the much more complicated optimized effective potential method, while obtaining about the same SCF accuracy. In the tLap functional, the variables to differentiate upon are  $n_\sigma$ ,  $\tau_\sigma$ , and  $\nabla^2 n_\sigma$ .

### 3 Computational Details

All calculations were done with the Q-Chem program, 3.1 release [11], using the exhaustive G3 basis set G3LARGE [12,13]. An atom-centered grid is used for the numerical integration based on the Becke’s relative weight scheme [14]. The radial part of the grid is treated by the Euler-Maclaurin scheme proposed by Murray et al. [15] and the angular part by Lebedev quadrature [16]. Unpruned grid with 128 radial and 194 angular points is maintained throughout all calculations. Single-determinantal Kohn-Sham state converged to integer orbital occupancies is employed to represent the ground state of atoms, in view of atomization energy estimates [6].

### 4 Results and Discussion

The validation of the new hybrid functional in comparison with some current top notched functionals is performed here based on the Lap test set <sup>6–8</sup>. The latter is more compact and faster than other established sets (G2, G3), while giving about the same qualitative answers. We follow the wisdom that a careful selection of diverse examples is more important than their overall number. The choice of the examples was based also on the availability of reliable reference data. The present test set consists of:

- (i) Thermochemistry and geometry of 20 diatomic and 19 polyatomic molecules, most of which are difficult at least for GGA:  
H<sub>2</sub>, N<sub>2</sub>, F<sub>2</sub>, O<sub>2</sub>, S<sub>2</sub>, P<sub>2</sub>, Cl<sub>2</sub>, HF, CO, NO, PN, CN, NH, CS, CH, OH, HCl, SiO, NaCl, NaF,  
HCN, H<sub>2</sub>O, H<sub>2</sub>S, CO<sub>2</sub>, NH<sub>3</sub>, PH<sub>3</sub>, N<sub>2</sub>O, H<sub>2</sub>O<sub>2</sub>, SiH<sub>4</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, H<sub>2</sub>CO, CH<sub>3</sub>OH, C<sub>6</sub>H<sub>6</sub>, trans-butadiene (C<sub>4</sub>H<sub>6</sub>), pyrrole (C<sub>4</sub>H<sub>5</sub>N), pyridine (C<sub>5</sub>H<sub>5</sub>N)
- (ii) Transition metal mono-carbonyls having difficult for DFT metal-ligand bonding.
- (iii) Energy barriers of selected reactions that are very difficult to describe quantitatively.

The parameter optimization of B3tLap was done on a subset of 18 molecules from set (i) only.

#### 4.1 Atomization energy and geometry of molecules

Table 1 contains our results of atomization energy and geometry data. The notation “B” denotes the GGA exchange of Becke (1988). Results from some other functionals, BLYP [10,17], BLap3 [7], BtLap [10,6], B3LYP [1,2], BMK [18],

Table 1. Mean absolute errors (MAE) for atomization energies  $D_e$  (kcal/mol) and bond lengths  $R_e$  (Å)

| XC     | MAE for $D_e$       |            |                  | MAE for $R_e$       |            |           |
|--------|---------------------|------------|------------------|---------------------|------------|-----------|
|        | Diatomic            | Polyatomic | All 39 molecules | Diatomic            | Polyatomic | All bonds |
|        | XC with no HF exch. |            |                  | XC with no HF exch. |            |           |
| BLYP   | 5.58                | 5.23       | 5.41             | 0.0174              | 0.0112     | 0.0140    |
| B3Lap  | 3.30                | 8.39       | 5.78             | 0.0189              | 0.0080     | 0.0132    |
| BtLap  | 3.08                | 3.81       | 3.44             | 0.0155              | 0.0105     | 0.0127    |
|        | XC with HF exch.    |            |                  | XC with HF exch.    |            |           |
| BMK    | 2.72                | 2.49       | 2.61             | 0.0112              | 0.0081     | 0.0095    |
| M06    | 2.69                | 2.57       | 2.63             | 0.0083              | 0.0081     | 0.0082    |
| B3LYP  | 2.51                | 1.82       | 2.17             | 0.0073              | 0.0046     | 0.0058    |
| B3tLap | 2.04                | 2.13       | 2.08             | 0.0110              | 0.0085     | 0.0096    |

M06 [4,5], are also included for comparison. Among the ‘pure DFT’ functionals, the meta-GGA scheme BtLap is a definite improvement over B3Lap and BLYP, the latter considered as one of the best GGA. It is reasonable to expect that the better a pure DFT scheme, the better would be its hybrid extension. Indeed, the new B3tLap functional is slightly more accurate here than B3LYP, M06, and BMK regarding atomization energies. Concerning bond lengths, the inclusion of HF exchange greatly improves the accuracy, comparing BLYP vs. B3LYP and BtLap vs. B3tLap. B3LYP gives here the smallest mean absolute error (MAE) of bond lengths followed closely by M06, BMK and B3tLap. The inclusion of the electron kinetic energy density as a non local variable may (BtLap) or may not (B3Lap) improve the model chemistry compared to say, GGA (BLYP). It all depends on the details of the functional employing these variables. Inclusion of a small fraction of HF exchange definitely improves the model chemistry, and a comparison of BtLap with B3tLap confirms once more this fact.

#### 4.2 Weak transition metal-ligand bonding

This type of bonding is often difficult to describe quantitatively, due to strong static correlation effects. Table 2 contains results for three weakly bound transition-metal carbonyls, CuCO, CrCo, and FeCO. Most GGA functionals tend to overestimate significantly the bond strength here [8,19-20]. The GGA BP (Becke (88) exchange [10] – Perdew (86) correlation [22]) overestimates the binding by about a factor of three. Similar are the estimates with other GGA like PW91 and PBE (not included in the table). The meta-GGA functional BtLap leads to some improvement here. A fraction of HF exchange helps further as far as the binding energy concern, comparing the BtLap with B3tLap results, Table 2. Overall B3tLap and B3LYP perform about the same here and are better than the rest of the functionals tested on these three mono-carbonyls. M06 is doing not bad on Cu–CO and Cr–Co, but meets some problems with the Fe–CO bond. While improving the bond energies, hybrid functionals do not necessarily improve the vibrational frequencies in these carbonyls [20]. The assessment of

Table 2. Transition metal-ligand bonding in mono-carbonyls

|                                       | BP     | BtLap  | B3LYP  | B3tLap | M06    | expt <sup>a</sup> |
|---------------------------------------|--------|--------|--------|--------|--------|-------------------|
| Cu-CO (2S+1=2)                        |        |        |        |        |        |                   |
| $D_0$ (kcal/mol)                      | 17.5   | 9.6    | 7.3    | 5.5    | 7.4    | 6±1.2             |
| $R_{O-C}$ (Å)                         | 1.1563 | 1.1539 | 1.1402 | 1.1417 | 1.1365 |                   |
| $R_{Cu-C}$ (Å)                        | 1.8828 | 1.9506 | 1.9578 | 1.9829 | 1.9786 |                   |
| $\nu(\text{CO})$ (cm <sup>-1</sup> )  | 1964.2 | 1979.3 | 2047.5 | 2058.3 | 2089.1 | 2010              |
| $\nu(\text{M-C})$ (cm <sup>-1</sup> ) | 409.8  | 350.1  | 333.8  | 311.6  | 327.3  |                   |
| Cr-CO (2S+1=7)                        |        |        |        |        |        |                   |
| $D_0$ (kcal/mol)                      | 11.4   | 4.6    | 4.6    | 2.1    | 4.0    | 2.5-4.5           |
| $R_{O-C}$ (Å)                         | 1.1591 | 1.1542 | 1.1427 | 1.1412 | 1.1389 |                   |
| $R_{Cr-C}$ (Å)                        | 2.1349 | 2.2565 | 2.2035 | 2.2970 | 2.2025 |                   |
| $\nu(\text{CO})$ (cm <sup>-1</sup> )  | 1931.8 | 1966.5 | 2021.5 | 2056.2 | 2065.4 | 1977              |
| $\nu(\text{M-C})$ (cm <sup>-1</sup> ) | 327.4  | 249.1  | 274.3  | 211.5  | 291.6  |                   |
| Fe-CO (2S+1=3)                        |        |        |        |        |        |                   |
| $D_0$ (kcal/mol)                      | 30.2   | 16.3   | 8.6    | 8.5    | 18.3   | 10.5±3.5          |
| $R_{O-C}$ (Å)                         | 1.1697 | 1.1716 | 1.1485 | 1.1506 | 1.1608 |                   |
| $R_{Fe-C}$ (Å)                        | 1.7029 | 1.7462 | 1.7693 | 1.8004 | 1.7384 |                   |
| $\nu(\text{CO})$ (cm <sup>-1</sup> )  | 1941.9 | 1907.0 | 2030.7 | 2037.7 | 2012.5 | 1982±10           |
| $\nu(\text{M-C})$ (cm <sup>-1</sup> ) | 566.1  | 517.0  | 459.4  | 443.8  | 558.2  | 530±10            |

<sup>a</sup>Data from Ref. 20.

the theoretical bond lengths is somewhat obscure due to the lack of reliable experimental data [20]. The calculated metal-ligand bond lengths vary noticeably from one functional to another, the GGA yielding much shorter metal-ligand bonds than the meta-GGA and hybrid functionals. B3tLap yields somewhat longer meta-ligand bonds compared to B3LYP and M06. Accurate experimental estimates of the equilibrium bond lengths here are necessary, in order to complete the assessment.

### 4.3 Reaction barriers of some difficult reactions

In Table 3 we present calculated classical energy barriers for 18 reactions (ten entries, eight of which have distinct forward and reverse reaction barriers) from the Truhlar's data base<sup>1</sup>. All these are known to be very difficult to describe with density functionals. They involve a hydrogen abstraction via a transition state with strong spin-charge fluctuations [22] and strong static correlation [23]. The early meta-GGA functional BLap3 [7] has been found useful in the past for such type of reactions [24,25]. The more recent meta-GGA-hybrid functionals BMK and M06 have been carefully parameterized (17 parameters) including such reactions in the training set. These two functionals show the smallest MAE here (1.6 kcal/mol and 1.5 kcal/mol respectively), by about 1 kcal/mol larger than the MAE of the CCSD(T) benchmark. B3tLap gives MAE of 2.9 kcal/mol, compared to the MAE of 5.5 kcal/mol for B3LYP. No reaction barriers have

<sup>1</sup>Truhlar's online database: <http://comp.chem.umn.edu/database>

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Table 3. Energy barriers (kcal/mol) for selected ‘difficult’ reactions (f = forward, r = reverse reaction)

| Reaction  |                             | B3LYP      | B3tLap     | BMK        | M06        | CCSD(T)<br>//QCISD <sup>a</sup> | Ref. <sup>b</sup> |
|---|-----------------------------|------------|------------|------------|------------|---------------------------------|-------------------|
| H + HCl ↔ H <sub>2</sub> + Cl                               | V <sub>f</sub> <sup>#</sup> | 0.7        | 3.8        | 4.1        | 6.5        | 5.2                             | <b>5.7</b>        |
|   | V <sub>r</sub> <sup>#</sup> | 4.4        | 6.3        | 5.5        | 4.0        | 8.9                             | <b>8.7</b>        |
| H + HCl ↔ HCl + H   | V <sub>f</sub> <sup>#</sup> |            |            |            |            |                                 |                   |
|   | V <sub>r</sub> <sup>#</sup> | 12.7       | 16.3       | 17.0       | 17.4       | 18.9                            | <b>18.0</b>       |
| H + OH ↔ H <sub>2</sub> + O                                 | V <sub>f</sub> <sup>#</sup> | 4.0        | 7.3        | 10.1       | 9.2        | 9.9                             | <b>10.7</b>       |
|   | V <sub>r</sub> <sup>#</sup> | 6.2        | 9.0        | 10.5       | 10.7       | 13.8                            | <b>13.1</b>       |
| F + H <sub>2</sub> ↔ HF + H                                 | V <sub>f</sub> <sup>#</sup> | -5.6       | -3.6       | -1.8       | 3.4        | 1.8                             | <b>1.8</b>        |
|   | V <sub>r</sub> <sup>#</sup> | 23.2       | 26.8       | 29.7       | 31.3       | 32.4                            | <b>33.4</b>       |
| H + H <sub>2</sub> ↔ H <sub>2</sub> + H                     | V <sub>f</sub> <sup>#</sup> |            |            |            |            |                                 |                   |
|   | V <sub>r</sub> <sup>#</sup> | 4.3        | 7.5        | 9.7        | 8.4        | 9.8                             | <b>9.6</b>        |
| OH + H <sub>2</sub> ↔ H + H <sub>2</sub> O                  | V <sub>f</sub> <sup>#</sup> | 0.8        | 3.1        | 4.2        | 2.3        | 5.5                             | <b>5.1</b>        |
|   | V <sub>r</sub> <sup>#</sup> | 13.3       | 17.4       | 20.4       | 20.4       | 20.5                            | <b>21.2</b>       |
| OH + NH <sub>3</sub> ↔ H <sub>2</sub> O + NH <sub>2</sub>   | V <sub>f</sub> <sup>#</sup> | -2.3       | -0.5       | 2.9        | 1.5        | 3.2                             | <b>3.2</b>        |
|   | V <sub>r</sub> <sup>#</sup> | 7.2        | 8.9        | 11.9       | 12.8       | 12.7                            | <b>12.7</b>       |
| H + H <sub>2</sub> S ↔ HS + H <sub>2</sub>                  | V <sub>f</sub> <sup>#</sup> | -0.4       | 2.6        | 3.5        | 4.0        | 3.6                             | <b>3.5</b>        |
|   | V <sub>r</sub> <sup>#</sup> | 15.9       | 16.5       | 16.6       | 17.0       | 18.2                            | <b>17.3</b>       |
| O + HCl ↔ OH + Cl   | V <sub>f</sub> <sup>#</sup> | 1.5        | 4.2        | 7.2        | 9.9        | 10.7                            | <b>9.8</b>        |
|   | V <sub>r</sub> <sup>#</sup> | 4.4        | 5.0        | 8.1        | 6.0        | 10.4                            | <b>10.4</b>       |
| H + CH <sub>3</sub> OH ↔ H <sub>2</sub> +CH <sub>2</sub> OH | V <sub>f</sub> <sup>#</sup> | 3.7        | 6.7        | 9.4        | 8.6        | 9.6                             | <b>7.3</b>        |
|   | V <sub>r</sub> <sup>#</sup> | 13.2       | 14.1       | 14.9       | 13.7       | 15.5                            | <b>13.8</b>       |
| MAE on 18 reactions   |                             | <b>5.5</b> | <b>2.9</b> | <b>1.6</b> | <b>1.5</b> | <b>0.5</b>                      |                   |

<sup>a</sup>CCSD(T) results available online from the Truhlar’s data base.

<sup>b</sup>Best available reference value for each reaction (from the Truhlar’s data base).

been included in the parameter optimization of either B3tLap (5 parameters), or B3LYP (8 parameters). We are planning some re-parametrization of the B3tLap functional to see if we could improve it further for reaction barriers without deteriorating the rest of its model chemistry.

## 5 Conclusions

The recently developed meta-GGA correlation functional tLap is used here to obtain the new meta-GGA-hybrid combination B3tLap. The validation on the Lap tests set shows that B3tLap has some promises in maintaining a robust and high accuracy for diverse systems. For applications to catalysis this is particularly important, especially concerning transition-metal chemistry and reaction kinetics. B3tLap is slightly more accurate than B3LYP, BMK and M06 for atomization energies and weak transition-metal ligand bonding, and definitely more accurate than B3LYP for reaction barriers. We hope to be able soon to present

also validation on solid state applications, the development of the corresponding code for this purpose is ongoing.

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