Revisiting the gradient expansion in meta-GGAs: Energetic binding and band gaps

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ABSTRACT

Over the past decade, meta-GGAs have made great progress, offering almost hybrid accuracy at almost GGA computational cost. Meta-GGAs like B97M-V and SCAN are very accurate for e.g. energetic binding. On the other hand, we have recently shown that the meta-GGA TASK predicts the right band gaps for the right reason [1].

In our contribution, we aim to achieve state-of-the-art accuracy for both energetic binding and band gaps within a single non-empirical meta-GGA. To this end, we reconsider the gradient expansion for meta-GGAs. In meta-GGAs, both the (reduced) gradient of the density s and the kinetic energy density τ contribute to the gradient expansion. Since its dependence on τ determines the degree of nonlocality in a meta-GGA, adjustment of the relative contributions from s and τ allows for a balanced treatment of energetic binding and nonlocal features of the potential. To demonstrate this, we construct the non-empirical meta-GGA LAK based on a thoughtful partition of the gradient expansion in s and τ. Table 1 compares LAK with PBE, SCAN, and HSE06.

Table 1: Mean absolute error for 6 main-group atomization energies, 20 main-group bond lengths, 20 lattice constants of solids, 22 interaction energies of weakly bound complexes, and 15 semi-conductor band gaps.

	AE6 (kcal/mol)	MGBL20 (Å)	LC20 (Å)	S22 (kcal/mol)	scBG15 (eV)
PBE	14.3	0.009	0.055	2.43	0.91
SCAN	3.3	0.005	0.015	0.81	0.59
LAK	3.5	0.003	0.054	0.55	0.18
HSE06	4.5	0.006	0.032	2.20	0.17

References

[1] Lebeda, T. et al. Right band gaps for the right reason at low computational cost with a meta-GGA. *Phys. Rev. Mater.* **2023**, *7*, 093803; *Phys. Rev. Res.* **2022**, *4*, 023061.