

HOW FAR CAN WE GO WITH SEMILOCAL DENSITY FUNCTIONALS, AND HOW CAN WE GO BEYOND THEM?

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WHAT IS DENSITY FUNCTIONAL THEORY?

KOHN-SHAM DENSITY FUNCTIONAL THEORY HAS GROWN UP IN 50 YEARS TO BECOME THE MOST WIDELY-USED METHOD OF ELECTRONIC STRUCTURE CALCULATION IN PHYSICS AND CHEMISTRY, AND THE LYNCH-PIN OF THE MATERIALS GENOME INITIATIVE.

IT REDUCES THE PROBLEM OF FINDING GROUND-STATE ENERGIES AND ELECTRON DENSITIES TO A SELF-CONSISTENT ONE-ELECTRON PROBLEM, IN A WAY THAT IS IN PRINCIPLE EXACT.

THIS THEORY PREDICTS NOT ONLY THE GROUND-STATE ENERGY AND DENSITY OF AN ATOM, MOLECULE, OR SOLID, BUT ALSO (WITHIN THE BORN-OPPENHEIMER APPROXIMATION) THE FORCES ON THE NUCLEI, THEIR EQUILIBRIUM POSITIONS (STRUCTURE), AND THEIR VIBRATIONAL FREQUENCIES.

IT IS A WAY OF DOING QUANTUM MECHANICS FOR INTERACTING ELECTRONS WITHOUT A CORRELATED MANY-ELECTRON WAVEFUNCTION.

IN PRACTICE, ONE MUST APPROXIMATE THE EXCHANGE-CORRELATION ENERGY AS A FUNCTIONAL OF THE ELECTRON DENSITY (A RULE THAT TAKES US FROM THE DENSITY AS A FUNCTION OF POSITION TO AN ENERGY).

WHAT IS THE EXCHANGE-CORRELATION ENERGY?

IT IS A NEGATIVE TERM IN THE TOTAL ENERGY THAT DESCRIBES HOW MUCH THE ENERGY (MAINLY THE COULOMB PART) IS LOWERED DUE TO THE FACT THAT ONE ELECTRON AVOIDS A CLOSE APPROACH TO ANOTHER, AS A CONSEQUENCE OF THE FERMION ANTISYMMETRY (EXCHANGE) AND THE COULOMB REPULSION (CORRELATION).

AN ELECTRON AT A GIVEN POSITION IS SURROUNDED BY A “PERSONAL SPACE” OR XC HOLE FROM WHICH OTHER ELECTRONS ARE EXCLUDED.

THIS TERM PRODUCES MOST OF THE BINDING OF ONE ATOM TO ANOTHER, TO FORM MOLECULES AND SOLIDS. THIS HAPPENS BECAUSE, AS ONE ATOM APPROACHES ANOTHER, IT HAS MORE OPPORTUNITY TO AVOID OTHER ELECTRONS.

WHAT IS A SEMILOCAL DENSITY FUNCTIONAL?

IT IS AN APPROXIMATION THAT TAKES THE FORM OF A SINGLE INTEGRAL OVER THREE-DIMENSIONAL SPACE OF A FUNCTION OF ARGUMENTS THAT, IN A KOHN-SHAM CALCULATION, ARE READILY AVAILABLE AT EACH POSITION IN THAT SPACE, SUCH AS THE ELECTRON DENSITY, ITS GRADIENT, OR THE ORBITAL KINETIC ENERGY DENSITY OF THE FICTITIOUS AUXILIARY SYSTEM OF NON-INTERACTING ELECTRONS.

THE SINGLE INTEGRATION OVER A GRID MAKES SEMILOCAL APPROXIMATIONS COMPUTATIONALLY EFFICIENT, AND THUS THE METHOD OF CHOICE FOR LARGE MOLECULES OR UNIT CELLS, *AB INITIO* MOLECULAR DYNAMICS, ETC.

SEMILOCAL APPROXIMATIONS INCLUDE THE LOCAL SPIN DENSITY APPROXIMATION (LSDA), THE GENERALIZED GRADIENT APPROXIMATION (GGA), AND THE META-GGA.

HOW ARE SEMILOCAL APPROXIMATIONS CONSTRUCTED WITHOUT EMPIRICAL FITTING BY THE METHOD OF CONSTRAINT SATISFACTION?

WE KNOW OR CAN DERIVE MANY EXACT PROPERTIES OF THE EXCHANGE-CORRELATION ENERGY AS A FUNCTIONAL OF THE DENSITY.

SEMILOCAL APPROXIMATIONS CAN BE CONSTRUCTED TO SATISFY THESE “EXACT CONSTRAINTS”. WE CAN SATISFY MORE EXACT CONSTRAINTS BY STARTING FROM THE LOCAL DENSITY ARGUMENT (LSDA), ADDING THE DENSITY GRADIENT ARGUMENT (GGA), THEN ADDING THE ORBITAL KE DENSITY ARGUMENT (META-GGA).

WHEN SHOULD SEMILOCAL FUNCTIONALS WORK?

BOTH THESE CONDITIONS MUST BE SATISFIED:

- (1) WHEN THE REAL SYSTEM HAS AN EXACT EXCHANGE-CORRELATION HOLE THAT IS WELL-LOCALIZED AROUND ITS ELECTRON, EITHER BECAUSE THE EXACT EXCHANGE HOLE IS LOCALIZED (AS IN ATOMS or SLOWLY-VARYING DENSITIES) OR BECAUSE THE DELOCALIZATION OF THE EXACT EXCHANGE HOLE IS WELL-CANCELLED BY THE DELOCALIZATION OF THE EXACT CORRELATION HOLE (CANCELLATION OF ERROR BETWEEN SEMILOCAL X AND SEMILOCAL C IN TYPICAL MOLECULES AND SOLIDS NEAR EQUILIBRIUM GEOMETRIES).
- (2) WHEN THE SELFCONSISTENT DENSITY FROM THE SEMILOCAL APPROXIMATION DOES NOT SHOW LARGE SPURIOUS CHARGE TRANSFERS BETWEEN CHEMICALLY-DIFFERENT SPECIES.

OUR STRATEGY TO BUILD MORE-ACCURATE FUNCTIONALS:

FIRST FIND THE BEST SEMILOCAL FUNCTIONAL BY SATISFYING ALL THE EXACT CONSTRAINTS THAT A SEMILOCAL FUNCTIONAL CAN. (SCAN!)

THEN IMPOSE CONSTRAINTS THAT ONLY A NONLOCAL FUNCTIONAL THAT CAN SATISFY:

- (a) LONG-RANGE VAN DER WAALS INTERACTIONS
- (b) SELF-INTERACTION CORRECTIONS, WHICH MAKE THE APPROXIMATION EXACT FOR ALL ONE-ELECTRON DENSITIES AND BETTER FOR FRACTIONAL CHARGE TRANSFERS BETWEEN NUCLEAR CENTERS.

**STRONGLY CONSTRAINED AND APPROPRIATELY
NORMED (SCAN) META-GENERALIZED
GRADIENT APPROXIMATION FOR EXCHANGE
AND CORRELATION**

**Jianwei Sun, Adrienn Ruzsinszky, & John P. Perdew
Physical Review Letters 115, 036402 (2015)**

intended as an accurate & efficient density functional

THERE IS A FIVE-RUNG LADDER OF APPROXIMATIONS, IN WHICH EACH RUNG ADDS A NEW INGREDIENT TO THE ENERGY DENSITY. THE FIRST THREE RUNGS ARE COMPUTATIONALLY SEMILOCAL AND THUS EFFICIENT, AND CAN BE NON-EMPIRICAL. THEY ARE NEEDED FOR:

LARGE SYSTEMS,
LONG-TIME MOLECULAR DYNAMICS SIMULATIONS,
HIGH-THROUGHPUT MATERIALS SEARCHES.

LOCAL SPIN DENSITY APPROXIMATION (LSDA) (E.G., PERDEW-WANG OR PW92)

GENERALIZED GRADIENT APPROXIMATION (GGA): (E.G., PERDEW-BURKE ERNZERHOF OR PBE96)

META-GGA (MGGA): (E.G., TAO-PERDEW-STAROVEROV-SCUSERIA OR TPSS03, SCAN)

THE FOURTH RUNG OF HYBRID FUNCTIONALS WITH EXACT EXCHANGE CAN BE MUCH MORE EXPENSIVE.

WHY GO BEYOND OUR NONEMPIRICAL TPSS META-GGA?

- (1) WE RECENTLY DERIVED A TIGHT BOUND ON THE EXCHANGE ENERGY, WHICH TPSS AND MOST PREVIOUS GGA'S AND META-GGA'S VIOLATE STRONGLY. THERE ARE ALSO OLDER EXACT CONSTRAINTS (E.G., NONUNIFORM DENSITY SCALING) WHICH TPSS VIOLATES. WE INTEND TO SATISFY ALL 17 KNOWN EXACT CONSTRAINTS THAT A META-GGA CAN SATISFY.
- (2) TPSS IS LESS ACCURATE THAN PBE FOR THE CRITICAL PRESSURES OF STRUCTURAL PHASE TRANSITIONS OF SOLIDS.
- (3) NEITHER TPSS NOR PBE PREDICT THE CORRECT INTERSTITIAL FORMATION ENERGY FOR SOLID SILICON.
- (4) IN HINDSIGHT: TPSS DOES NOT DESCRIBE INTERMEDIATE-RANGE VAN DER WAALS INTERACTION.

INTRODUCTION TO META-GGA

EFFICIENT SEMILOCAL APPROXIMATIONS TO E_{xc} :

$$E_{xc}[n_{\uparrow}, n_{\downarrow}] = \int d^3r n \varepsilon_{xc}(n_{\uparrow}, n_{\downarrow}, \nabla n_{\uparrow}, \nabla n_{\downarrow}, \tau_{\uparrow}, \tau_{\downarrow})$$

- LSDA: $n_{\sigma} = \sum_i^{occup} |\psi_{i,\sigma}|^2$
- GGA: ADDS ∇n_{\uparrow} AND ∇n_{\downarrow}
- MGGA: ADDS $\tau_{\sigma} = \sum_i^{occup} \frac{1}{2} |\nabla \psi_{i,\sigma}|^2$
- $\psi_{i,\sigma}$: KOHN – SHAM ORBITALS

THE ROLE OF τ (SPIN SUPPRESSED)

• LIMITING FORMS:

• SINGLE-ORBITAL SYSTEMS:

$$\tau^w = \frac{1}{8} |\nabla n|^2 / n$$

• UNIFORM ELECTRON GAS (UEG):

$$\tau^{unif} = \frac{3}{10} (3\pi^2)^{2/3} n^{5/3}$$

RIGHT DIMENSIONLESS INGREDIENTS FOR MGGA: $\alpha = \frac{\tau - \tau^w}{\tau^{unif}}$ (DDSOS)

REGION	α
SINGLE ORBITAL (COVALENT)	0
SLOWLY-VARYING DENSITY (METALLIC)	~ 1
OVERLAP OF CLOSED SHELLS (NONCOVALENT)	$\gg 1$

BASIC IDEAS AND GOALS OF SCAN

- BASIC IDEAS

- MODEL $\varepsilon_{x/c}^0$ FOR SINGLE-ORBITAL REGIONS ($\alpha = 0$) AND $\varepsilon_{x/c}^1$ FOR SLOWLY-VARYING REGIONS ($\alpha \approx 1$), RESPECTIVELY, AND USE $f_{x/c}(\alpha)$ TO INTERPOLATE BETWEEN THEM AND EXTRAPOLATE TO $\alpha \rightarrow \infty$.
- SATISFY AS MANY (17) EXACT CONSTRAINTS AS POSSIBLE (INCLUDING ALL CONSTRAINTS SATISFIED BY PBE)
- NORM OR FIT APPROPRIATELY

- GOALS

- ACCURATE FOR SYSTEMS WHERE XC HOLES ARE LOCALIZED
- SYSTEMATIC IMPROVEMENT OVER PBE
- CONSISTENT AND BALANCED PERFORMANCE FOR MOLECULES AND SOLIDS

APPROPRIATE NORMS: GUIDING SCAN FROM $\alpha=0$ TO $\alpha=1$, THEN TO $\alpha \rightarrow \infty$

- APPROPRIATE NORMS: **SYSTEMS WITH LOCALIZED XC HOLES** (SUFFICIENT IF X HOLES ARE LOCALIZED)
 - UNIFORM ELECTRON GAS AND H
 - **RARE-GAS ATOMS**
 - **THREE COEFFICIENTS** OF LARGE-Z LIMIT OF THE EXCHANGE AND CORRELATION ENERGIES OF NEUTRAL ATOMS
 - $\lim_{Z \rightarrow \infty} E_x(Z) = E_x^{LDA} + \gamma_{x1}Z + \gamma_{x2}Z^{2/3}$
 - $\lim_{Z \rightarrow \infty} E_c(Z) = E_c^{LDA} + \gamma_{c1}Z$
 - **Ar₂ AT COMPRESSED BOND LENGTHS** (1.6, 1.8, and 2.0 Å)
 - **JELLIUM SURFACE**

RELATIVE ERRORS (%) IN EX, EC, AND EXC OF RARE GAS ATOMS

	Ne	Ar	Kr	Xe
EX	-0.46	-0.26	-0.20	-0.07
EC	11.85	4.50	5.09	3.38
EXC	-0.07	-0.15	-0.09	-0.01

RELATIVE ERRORS IN EX OF Ar₂ AT DIFFERENT BOND LENGTHS, **WHERE THE REPULSIVE ENERGIES ARE ABOUT 100~300 KCAL/MOL**

R	1.6	1.8	2.0
REL ERROR (%)	-0.28	-0.26	-0.26

RELATIVE ERRORS IN JELLIUM SURFACE EXCHANGE-CORRELATION ENERGIES OF DIFFERENT DENSITIES. **NOTE ONLY $r_s=4$ IS USED FOR THE DETERMINATION OF THE PARAMETERS**

r_s	2	3	4	6
REL ERROR (%)	-0.2	-0.0	-0.0	4.1

RESULTS FOR MOLECULES AND SOLIDS

		G3 (kcal/mol)		BH76 (kcal/mol)		S22 (kcal/mol)		LC20 (Å)	
		ME	MAE	ME	MAE	ME	MAE	ME	MAE
GGA	BLYP	3.8	9.5	-7.9	7.9	-8.7	8.8		
	PBEsol	-58.7	58.8	-11.5	11.5	-1.3	1.8	-0.012	0.036
	PBE	-21.7	22.2	-9.1	9.2	-2.8	2.8	0.051	0.059
MGGA	SCAN	-4.6	5.7	-7.7	7.7	-0.9	0.9	0.007	0.016
	TPSS	-5.2	5.8	-8.6	8.7	-3.7	3.7	0.035	0.043
	M06L	-1.6	5.2	-3.9	4.1	-0.9	0.9	0.015	0.069

ME: MEAN ERROR;
MAE: MEAN ABSOLUTE
ERROR

LC20: LATTICE
CONSTANTS OF 20
SOLIDS INCLUDING
METALS,
SEMICONDUCTORS, AND
INSULATORS

G3: FORMATION ENERGIES OF 223 MOLECULES (AT THE ORDER OF 100~1000 KCAL/MOL) (REALLY ATOMIZATIONS)

BH76: 76 REACTION BARRIERS (AT THE ORDER OF 0~50 KCAL/MOL)

S22: 22 MOLECULAR COMPLEXES BOUND BY WEAK BONDS (AT THE ORDER OF 0~20 KCAL/MOL)

SUMMARY:

AS WE CLIMB THE LADDER FROM LSDA TO PBE TO SCAN:

ATOMIZATION ENERGIES, ENERGY BARRIERS, AND LATTICE CONSTANTS ALL IMPROVE. THE BINDING ENERGIES OF WEAKLY-BOUND COMPLEXES WORSEN FROM LSDA TO PBE, THEN IMPROVE DRAMATICALLY FROM PBE TO SCAN. LATTICE CONSTANTS ALSO IMPROVE DRAMATICALLY FROM PBE TO SCAN.

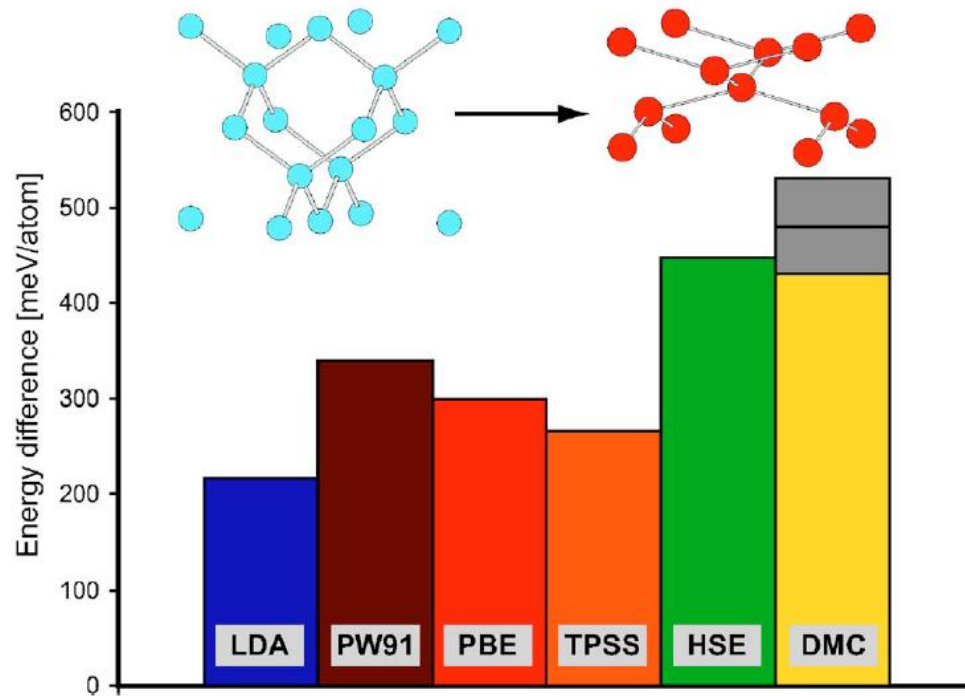
THE NONEMPIRICAL SCAN META-GGA IS MORE ACCURATE THAN THE NONEMPIRICAL TPSS META-GGA, ESPECIALLY FOR WEAK BONDS, PRESUMABLY BECAUSE SCAN SATISFIES MORE EXACT CONSTRAINTS AND APPROPRIATE NORMS.

NOTE THAT SCAN IS NOT FITTED TO ANY BONDED SYSTEM. THUS ITS RESULTS FOR BONDS ARE GENUINE PREDICTIONS, NOT FITS.

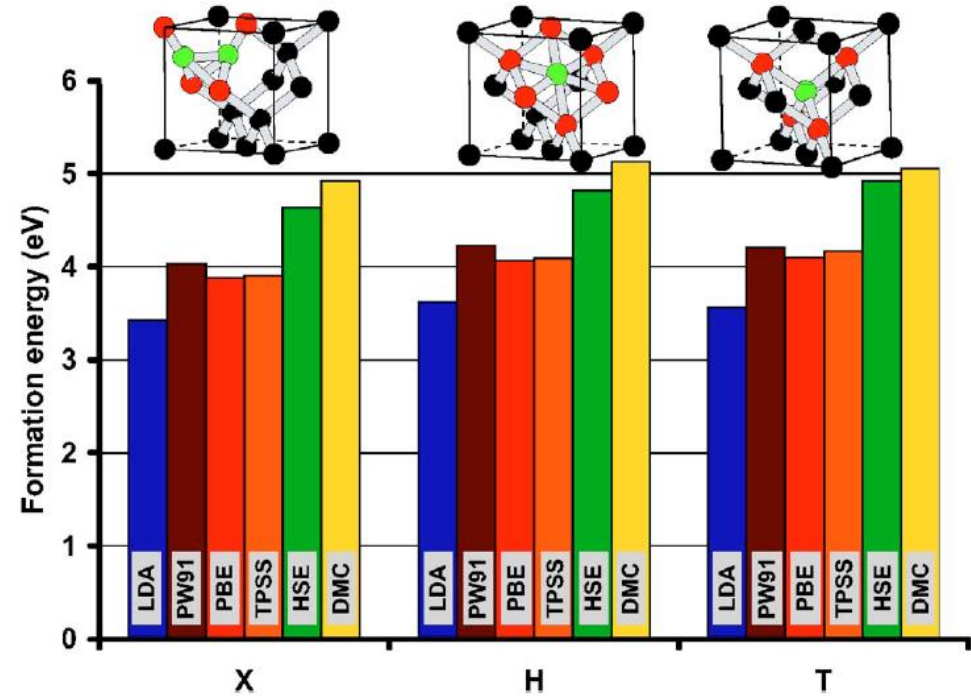
THE NONEMPIRICAL SCAN META-GGA IS MUCH MORE ACCURATE THAN THE EMPIRICAL META-GGA M06L (35 EMPIRICAL PARAMETERS) FOR LATTICE CONSTANTS, AS ACCURATE FOR ATOMIZATION ENERGIES AND WEAK-BOND ENERGIES, BUT LESS ACCURATE FOR ENERGY BARRIERS. HOWEVER, ENERGY BARRIERS ARISE AT TRANSITION STATES WITH ELECTRONS SHARED OVER STRETCHED BONDS, FOR WHICH SEMILOCAL FUNCTIONALS SHOULD NOT BE EXPECTED TO WORK.

Phase transition pressure and defect formation energies of Si: The situation before SCAN

STRUCTURAL PHASE TRANSITION



INTERSTITIAL DEFECT FORMATION ENERGY

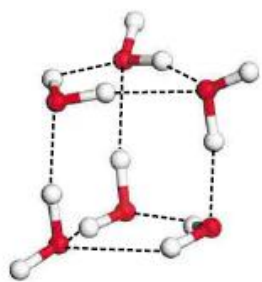


REF: E.R. Batista, *et al*, PRB, 74, 121102 (2006)

PERFORMANCE OF SCAN FOR SOLID Si

	Phase transition		Interstitial defect formation (eV)		
	δE (meV)	p_t (Gpa)	X	H	T
PBE	290	8.4	3.61	3.65	3.78
SCAN	411	14.3	4.29	4.36	4.59
Ref	480 ± 50	11-15	4.5-4.8		

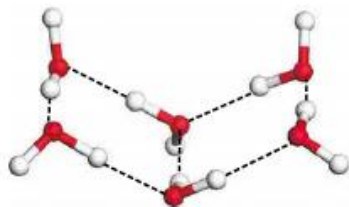
ENERGETIC ORDERING OF WATER HEXAMERS (BINDING ENERGY IN meV/H₂O)



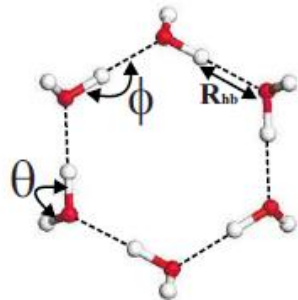
Prism



Cage



Book



Cyclic

method	Prism	Cage	Book	Cyclic
MP2	332.3	331.9	330.2	324.1
DMC	331.9	329.5	327.8	320.8
CCSD(T)	347.6	345.5	338.9	332.5
PBE	336.1	339.4	345.6	344.1
B3LYP	294.4	297.1	305.1	306.7
TPSS	303.9	302.8	313.6	316.7
SCAN	376.8	375.6	370.0	359.7
PBE+vd W(TS)	369.6	372.6	370.6	360.7

Ref: B. Santra, *et al*, JCP, **129**, 194111 (2008)

ALTHOUGH SCAN OVERBINDS ONE WATER MOLECULE TO ANOTHER, IT STILL PREDICTS THE CORRECT ENERGETIC ORDER OF THE FOUR WATER HEXAMERS. MOREOVER, FOR A FIXED NUMBER OF HYDROGEN BONDS, IT CORRECTLY PREDICTS THE ENERGY DIFFERENCES PER H₂O UNIT BETWEEN THESE CLUSTERS, AND BETWEEN THE DIFFERENT PHASES OF ICE. THIS SHOWS THAT SCAN CAPTURES MOST OF THE VAN DER WAALS INTERACTION IN WATER.

STABILITIES OF CRYSTAL STRUCTURES

Gerd Ceder found the wrong (alpha) ground-state crystal structure for MnO₂, using PBE and PBE+U.

Haowei Peng tried SCAN, and found the right (beta) ground-state crystal structure for this material, in agreement with experiment.

UNFORTUNATELY, SCAN IS NOT ALWAYS BETTER THAN PBE.

AN EXAMPLE IS THE DESORPTION ENERGY (eV) OF CO
FROM THE TOP SITE OF A Pt(111) SURFACE

LDA	PBE	SCAN	EXPT.
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2.3	1.7	1.9	1.4
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PERHAPS THIS IS A DENSITY-DRIVEN ERROR DUE TO A SPURIOUS TRANSFER OF
ELECTRONS FROM CO TO THE METAL SURFACE.

NEXT STEPS: NONLOCAL CORRECTIONS TO SCAN

- (1) FOR LONG-RANGE VAN DER WAALS INTERACTION
(SCAN+rVV10, ALREADY IMPLEMENTED).
- (2) FOR SELF-INTERACTION CORRECTION OR LOCAL HYBRID
(NEEDED FOR STRETCHED BONDS OR STRONG CORRELATION).

SUMMARY OF SCAN

- A META-GGA, STRONGLY CONSTRAINED AND APPROPRIATELY NORMED.
- COMPUTATIONALLY EFFICIENT AND NONEMPIRICAL.
- SYSTEMATIC IMPROVEMENT OVER THE PBE GGA AND PREVIOUS META-GGA's FOR A WIDE RANGE OF PROPERTIES FROM THE SCAN META-GGA.
- OFTEN PERFORMS LIKE A HYBRID FUNCTIONAL, AT LOWER COST AND WITH INTERMEDIATE-RANGE VAN DER WAALS INTERACTION.

WE EXPECT TO FIND MAJOR IMPROVEMENTS IN THE FORMATION ENERGIES AND THUS IN THE RELATIVE STABILITIES OF MOLECULES AND SOLIDS (EVEN WITHOUT NONLOCAL CORRECTIONS).

EXCHANGE

$$E_x^{SCAN}[n] = \int d^3rn \varepsilon_x^{unif}(n) F_x^{SCAN}(s, \alpha) \quad \varepsilon_x^{unif}(n) = -(3/4\pi)(3\pi^2 n)^{1/3} \quad s = \frac{|\nabla n|}{2(3\pi^2)^{1/3}(n)^{4/3}}$$

$$F_x^{SCAN}(s, \alpha) = \{h_x^1(s, \alpha) + f_x(\alpha)[h_x^0 - h_x^1(s, \alpha)]\}g_x(s)$$

EXACT CONSTRAINTS

1. TIGHT LOWER BOUND FOR EXCHANGE $F_x^{SCAN} \leq 1.174 \rightarrow h_x^0=1.174$

2. 4TH-ORDER GRADIENT EXPANSION OF SLOWLY VARYING DENSITY LIMIT ($s \rightarrow 0$ and $\alpha \rightarrow 1$):

$$F_x^{GE4}(s, \alpha) = 1 + \frac{10}{81}s^2 - \frac{1606}{18225}s^4 + \frac{511}{13500}s^2(1 - \alpha) + \frac{5913}{405000}(1 - \alpha)^2$$

RESUMMATION OF 4TH-ORDER GRADIENT EXPANSION (RGE):

$$h_x^1(s, \alpha) = 1 + k_1 - \frac{k_1}{1 + \frac{\mu_{AK}s^2(1 + b_4 s^2/\mu_{AK} \text{Exp}(-|b_4|s^2/\mu_{AK})) + \{b_1s^2 + b_2(1 - \alpha)\text{Exp}[-b_3(1 - \alpha)^2]\}}{k_1}}$$

$$\mu_{AK} = 10/81, b_1 = 0.156632, b_2 = 0.12083, b_3 = 0.5, b_4 = \frac{\mu_{AK}^2}{k_1} - 0.112654$$

3. NON-UNIFORM SCALING LIMIT: $\lim_{s \rightarrow \infty} F_x^{SCAN}(s, \alpha) \propto s^{-1/2} \rightarrow g_x(s) = 1 - \text{Exp}[-a_1s^{-1/2}] \quad a_1=4.9479: \text{Ex(H)}$

INTERPOLATION AND EXTRAPOLATION: $f_x(\alpha) = \text{Exp}\left[-\frac{c_{1x}\alpha}{1-\alpha}\right]\theta(1 - \alpha) - d_x \text{Exp}\left[\frac{c_{2x}}{1-\alpha}\right]\theta(\alpha - 1) \quad \theta(x): \text{STEP FUNCTION}$

UNDETERMINED PARAMETERS: k_1, c_{1x}, c_{2x}, d_x

NO CORRECTION TO RGE IN ANY POWER OF ∇n AT THE SLOWLY VARYING DENSITY LIMIT

CORRELATION

$$E_c^{SCAN}[n] = \int d^3r n \epsilon_c^{SCAN} \quad \epsilon_c^{SCAN} = \epsilon_c^1 + f_c(\alpha)(\epsilon_c^0 - \epsilon_c^1)$$

EXACT CONSTRAINTS

1. ONE ELECTRON SELF-CORRELATION FREE
 2. LOWER BOUND ON E_{xc} OF 2-ELECTRON DENSITIES: $E_{xc}[n] \geq 1.67 E_x^{LDA}$
 3. 2ND-ORDER GRADIENT EXPANSION OF SLOWLY VARYING DENSITY LIMIT → A SIMPLIFIED PBE CORRELATION FOR ϵ_c^1
 4. NON-POSITIVITY → $\epsilon_c^0 \geq \epsilon_c^1$
- NONEMPIRICAL ϵ_c^0

INTERPOLATION AND EXTRAPOLATION: $f_c(\alpha) = \text{Exp}\left[-\frac{c_{1c}\alpha}{1-\alpha}\right] \theta(1-\alpha) - d_c \text{Exp}\left[\frac{c_{2c}}{1-\alpha}\right] \theta(\alpha-1)$

UNDETERMINED PARAMETERS: c_{1c}, c_{2c}, d_c