术语表

波函数理论与近似

英文简称	中文术语	英文术语
	第一性	*ab initio*
WFT	波函数理论	wavefunction theory
SCF	自洽场	self-consistent field
post-HF	(专指波函数理论的) 后自洽场	post Hartree-Fock
	规范原点	gauge origin
RPA	无规相近似	random phase approximation
OO	轨道优化	orbital-optimized
SS	自旋相同	same-spin
OS	自旋相反	opposite-spin
SCS	自旋组分缩放	spin-component-scaled
PT	微扰	perturbation
CI	组态相互作用	configuration interaction
Full-CI	完全组态相互作用	full configuration interaction
CC	偶合簇	coupled-cluster
CEPA	耦合电子对近似	coupled electron pair approximation
CPF	耦合电子对泛函	coupled pair functional
IEPA	独立电子对近似	independent electron pair approximation
	(非) 限制性方法	(un)restricted
QMC	量子蒙特卡洛	quantum Monte Carlo
DMC	扩散蒙特卡洛	diffusion Monte Carlo
VMC	变分蒙特卡洛	variational Monte Carlo
	正交变换不变性	unitary invariance
	大小可延展性	size extensivity

密度泛函理论与近似

英文简称	中文术语	英文术语
DFT	密度泛函理论	density functional theory
DFA	密度泛函近似	density functional approximation
post-SCF	后自洽场	post self-consistent field
	无 (电子) 相互作用体系	noninteracting system
	N 可表示性	N-representability
xc	交换相关效应	exchange-correlation effect
LDA	局域密度近似	local density apprioximation
LSDA	局域密度近似	local spin-density apprioximation
GGA	广义梯度近似	generalized gradient approximation
meta-GGA	广义梯度的梯度近似	meta-generalized gradient approximation
hyb	杂化 (泛函)	hybrid (functional)
NL	离域	non-local
	半定域	semi-local
RSH	长短程分离杂化 (泛函)	range-separate hybrid (functional)
	局域混合 (泛函)	local hybrid (functional)
DH	双杂化 (泛函)	doubly hybrid (functional)
xDH	XYG3 型双杂化 (泛函)	XYG3-type doubly hybrid (functional)
bDH	B2PLYP 型双杂化 (泛函)	B2PLYP-type doubly hybrid (functional)
DSD	弥散矫正的 SCS DH	dispersion corrected SCS DH
AC	绝热路径	adiabatic connection
GLPT2	二阶 Görling-Levy 微扰	2^{nd}-order Görling-Levy perturbation
OEP	有效优化势	optimized effective potential

程序、技术、误差量标术语

英文简称	中文术语	英文术语
RI	恒等算符简化 (近似)	resolution-of-identity (approximation)
FPA		focal-point analysis
CBS	完备基组 (极限)	complete basis set (limit)
WTMAD-2	(GMTKN55) 第二型加权平均绝对值误差	weighted mean absolute deviation (scheme 2)
MEPUB	平均键绝对值误差	mean unsigned error per bond
DRAM	动态随机访问内存	dynamic random access memory
THC	张量超分解	tensor hyper-contraction

化学概念术语

英文简称	中文术语	英文术语
HOMO	最高占据分子轨道	highest occupied molecular orbital
LUMO	最低非占分子轨道	lowest unoccupied molecular orbital
HOMO/LUMO gap	HOMO 与 LUMO 能级差	energy gap between HOMO and LUMO

波函数方法

方法简称	方法全程	参考文献
HF	Hartree-Fock	1–3
MP*n*	*n*-th order Møller-Plesset perturbation	4
CCSD	coupled-cluster singles and doubles	5–6
CCSD(T)	CCSD with perturbative triplets	7
IEPA	independent electron-pair approximation	8–9
sIEPA	screened IEPA	10
MP2/cr	(scheme I of) corrected MP2	11

密度泛函方法

方法名称	提出年代	参考文献

原子轨道基组

基组家族	基组名称	基组基数 ζ	参考文献
Karlsruhe	def2-TZVPP	3	12–23
	def2-QZVPP	4	12–24
	def2-QZVPPD	4	12–25
	def2-universal-jkfit	(auxiliary)	23,26
	daug-def2-universal-jkfit	(auxiliary)	23,26–27
	def2-TZVPP-rifit	(auxiliary)	28–30
	def2-QZVPP-rifit	(auxiliary)	28–29
	def2-QZVPPD-rifit	(auxiliary)	28–31

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