术语表

英文简称	中文术语	英文术语
	第一性	*ab initio*
DFT	密度泛函理论	density functional theory
DFA	密度泛函近似	density functional approximation
WFT	波函数理论	wavefunction theory
SCF	自洽场	self-consistent field
post-SCF	后自洽场	post self-consistent field
post-HF	波函数理论 post-SCF	post Hartree-Fock
	规范原点	gauge origin
	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)
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

英文简称	中文术语	英文术语
DSD	弥散矫正的 SCS DH	dispersion corrected SCS DH
AC	绝热路径	adiabatic connection
RI	恒等算符简化 (近似)	resolution-of-identity (approximation)
CBS	完备基组 (极限)	complete basis set (limit)
FPA		focal-point analysis
QMC	量子蒙特卡洛	quantum Monte Carlo
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
CC	偶合簇	coupled-cluster
CI	组态相互作用	configuration interaction

电子结构方法与基组表

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

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