

Input parameters for the cluster 3D code

The Erlangen–Toulouse collaboratopm

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1 Input files

The cluster 3D code has the following input files:

<code>for005</code>	defines the qualifier <code><name></code> for the other <code>for005...</code> files
<code>for005.<name></code>	general input for settings, static and dynamics
<code>for005ion.<name></code>	ionic configuration of cluster
<code>for005surf.<name></code>	atomic configuration of substrate (optional)

The input for `for005.<name>` is sorted into namelists. They contain:

Namelist GLOBAL		in <code>for005.<name></code>
<i>choice of system</i>		
<code>kxbox</code>	nr. of grid points in x direction	
<code>kybox</code>	nr. of grid points in y direction	
<code>kzbox</code>	nr. of grid points in z direction	
	box sizes must fulfill $kxbox \geq kybox \geq kzbox$	
<code>numspin</code>	number of spin components (2=full spin treatment) (1=spin averaged, possible problem for ADSIC)	
<code>kstate</code>	maximum nr. of s.p. states which is possible (greater than <code>nclust</code>)	
<code>nclust</code>	number of QM electrons - if set to 0 or a negative value (charge) this will be automatically calculated $nclust = \sum_{i=1}^{n_{ion}} Z_{ion} = charge$, where Z_{ion} is charge of each ion	
<code>nion</code>	number of cluster ions	
<code>nspdw</code>	number of spin down electrons	
<code>nion2</code>	selects type of ionic background 0 \rightarrow jellium background 1 \rightarrow background from ionic pseudo-potentials 2 \rightarrow background read in from <code>potion.dat</code>	
<code>radjel</code>	Wigner-Seitz radius of jellium background	
<code>surjel</code>	surface thickness of jellium background	
<code>bbeta</code>	quadrupole deformation of jellium background	
<code>gamma</code>	triaxiality of jellium background	
<code>dx,dy,dz,</code>	grid spacing (in Bohr) for the 3D numerical grid - if negative this will be set to an optimal value and a value will be suggested for KXBOX in file NX - the code stops and has to be restarted the grid size is defined before compilation in <code>params.F90</code> it has to be correlant with pseudopotentials corresponds to <code>ecut</code> in solid state	
<code>rotclustx,y,z</code>	vector fo angle of initial rotation of ions	
<code>temp</code>	electronic temperature in static iteration	

Namelist GLOBAL		in for005.<name>
<i>initialization of wave functions</i>		
b2occ	deformation for initial harmonic oscillator wf's	
gamocc	triaxiality for initial harmonic oscillator wf's	
osfac	factor on initial oscillator radius	
deocc	nr. of states above Fermi energy (determines nr. of states)	
shiftWfX	shift of initial wavefunctions in x direction	
ishiftCMtoOrigin	switch to shift center of mass of cluster to origin	
ispinsep	initialize wavefunctiosn with some spin asymmetry	
init_lcao	choice of basis for wavefunction initialization	
	=0 \implies harmonic oscillator functions (center can be moved by shiftWfX)	
	=1 \implies atomic orbitals = WFs centered at ionic sites	
itback	nr. of iterations for jellium background	
<i>convergence issues</i>		
e0dmp	damping parameter for static solution of Kohn-Sham equations (typically about the energy of the lowest bound state)	
epswf	step size for static solution of Kohn-Shahm equations (of order of 0.5)	
epsoro	required variance to terminate static iteration (order of 10 ⁻⁵)	
occmix	mixing factor: new (thermal) occupation to old	
endcon	requires precision variance, termination criterion	
Namelist GLOBAL		in for005.<name>
<i>yet unsorted</i>		
tcoulfalr	switch to FALR Coulomb solver (else exact solver)	
dpolx	add stationary dipole field in x-direction	
dpoly	add stationary dipole field in y-direction	
dpolz	add stationary dipole field in z-direction	
scaleclustx	scaling of cluster configuration along x-axis	
scaleclusty	scaling of cluster configuration along y-axis	
scaleclustz	scaling of cluster configuration along z-axis	
scaleclust	if $\neq 1$: scaling of cluster configuration along x-y-z	
shiftclustx	shift of cluster configuration along x-axis	
shiftclusty	shift of cluster configuration along y-axis	
shiftclustz	shioft of cluster configuration along z-axis	
iswitch_interpol	switch to interpolated grid for PsP	
iplotorbitals	switch to print plot-file pOrbitals for all static states	

	Namelist DYNAMIC	in for005.<name>
<i>numerical and physical parameters for statics and dynamics</i>		
dt1	time step for propagating electronic wavefunctions, $\frac{\Delta t}{\Delta x^2} \leq 1$	
ismax	maximum number of static iterations	
idyniter	switch to s.p. energy as E0DMP for 'iter>idyniter'	
ifhamdiag	diagonalization of m.f. Hamiltonian in static step (presently limited to fully occupied configurations)	
isitmax	nr. of imaginary-time steps to improve static solution	
itmax	number of time steps for electronic propagation	
ifexpevol	exponential evolution 4. order instead of TV splitting	
iffastpropag	accelerated time step in TV splitting (for pure electron dynamics, interplay with absorbing b.c. ??)	
irest	switch to restart dynamics from file 'save'	
istat	switch to read wavefunctions from file 'rsave' it continues static iteration for 'ismax>0' it starts dynamics from these wf's for 'ismax=0'	
idenfunc	choice of density functional for LDA 1 → Perdew & Wang 1992 (default setting) 2 → Gunnarson & Lundquist 3 → only exchange in LDA	
isave	saves results after every 'isave' steps on file 'rsave' in and after static iteration on file 'save' in dynamic propagation	
ipseudo	switch for using pseudo-densities to represent substrate atoms	
ipsptype	type of pseudopotentials: 0 = soft local (errf); 1 = full Goedecker; 2 = local Goedecker; 3 = read from file goed.asci (no need to specify) ; 4 = semicore read from file goed.asci	
directenergy	.true. = direct computation of energy (only for LDA, Slater, KLI)	
ifsicp	selects type of self-interaction correction 0 = pure LDA, 1 = SIC-GAM, 2 = ADSIC; 3 = SIC-Slater; 4 = SIC-KLI; 5 = exact exchange; 6 = inactive; 7 = localized SIC; 8 = full SIC (double set). IFSICP=7 or 8 requires switch twostsic=1 in define.h . Option IFSICP=7 needs yet testing.	
icooltyp	type of cooling (0=none, 1=pseudo-dynamics, 2=steepest descent, 3=Monte Carlo)	
ifredmas	switch to use reduced mass for ions in dynamics	
ionmdtyp	ionic propagation (0=none, 1=leap-frog, 2=velocity Verlet)	
ntref	nr. time step after which absorbing bounds are deactivated	
nabsorb	number of absorbing points on boundary (0 switches off)	
powabso	power of absorbing boundary conditions	
ispherabso	switch to spherical mask in absorbing bounds	

	Namelist DYNAMIC	in for005.<name>
	<i>way of excitation</i>	
centfx	initial boost of electronic wavefuncftions in x-direction	
centfy	initial boost of electronic wavefuncftions in y-direction	
centfz	initial boost of electronic wavefuncftions in z-direction	
shiftinix	initial x-shift of electronic wavefunctions	
shiftiniy	initial y-shift of electronic wavefunctions	
shiftiniz	initial z-shift of electronic wavefunctions	
tempion	initial temperature of cluster ions	
ekmat	initial kinetic energy of substrate atom (boost in x , in eV)	
itft	choice of shape of laser pulse	
	1 = ramp laser pulse, sine switching on/off	
	2 = gaussian laser pulse	
	3 = \cos^2 pulse	
tnode	time (in fs) at which pulse computation starts	
deltat	length of ramp pulse ($itft = 1$), in fs	
tpeak	time (in fs, relative to $tnode$) at which peak is reached (for $itft = 1$ and 2, pulse length becomes $2*tpeak$)	
omega	laser frequency (in Ry)	
e0	laser field strength in Ry/Bohr	
e1x,e1y,e1z	orientation of pulse	
e0_2	field strength of second laser pulse (only $itft=3$)	
phase2	phase of second pulse	
omega2	frequency of second pulse	
tstart2	initial ime of second pulse	
tpeak2	peak time of 2. pulse (pulse length is $2*tpeak2$)	
iexcit	modus of excitation (0=shifts, 1=rotation)	
iangmo	switch to compute angular momentum	
irotat	axis of rotation for excitation (x=1,y=2,z=2,xyz=4)	
phirot	angle of rotation for excitation (in units of degree)	
phangle	angle of “rotation” into a $1ph$ state	
phphase	phase of “rotation” into a $1ph$ state	
nhstate,npstate	nr. of hole and particle state for $1ph$ excitation this $1ph$ option can only be run from $istat=1$	

	Namelist DYNAMIC	in for005.<name>
<i>flags for observables</i>		
iemomsRel	calculates multipole moments of electron density relative to origin (0) or c.m. of cluster (1)	
istinf	modulus for printing information in static iteration	
ifspemoms	switch to compute and print spatial s.p. moments	
iftransme	switch to compute and print transition m.elements	
irhoimt_time	modulus for printing slices of integrated densities	
jstinf	modulus for printing information in dynamic	
jinfo	modulus for printing dynamical information on infosp.<name>	
jdip	modulus for printing dipole moments on pdip.<name>	
jquad	modulus for printing quadrupole moments on pquad.<name>	
jesc	modulus for printing ionization pescel.<name>	
jdiporb	modulus for printing dipoles for s.p. states on pdiporb.xyz	
jenergy	modulus for printing energy information on penergies.<name>	
jener	modulus for printing ionic energies	
iflocaliz	activates computation of Becke's localization	
jelf	modulus for analyzing and printing electron localization in dynamics various files are written of the form pelf*.<name>	
iflocaliz	modulus for analyzing and printing electron localization in statics	
jstinf	modulus for printing s.p. energies and variances	
jpos	modulus for printing ionic positions on pposion.<name>	
jvel	modulus for printing ionic velocities on pvelion.<name>	
jstateoverlap	switch to compute overlap of static state with the state directly after dynamical initialization	
jforce	modulus for printing ionic forces	
jgeomion	modulus for printing global measures of ionic configuration	
jang	modulus for printing electronic angular momentum	
jangabso	modulus for printing angular distribution of emitted electrons	
jspdp	modulus for printing spin dipole momenta	
jposcm	modulus for printing electronic center of mass	
ipasinf	modulus for printing information on general observables	
jgeomel	modulus for printing global measures of electronic geometry	
jelf	modulus for evaluating and printing electron localization	
jmp	modulus for storing information for PES	
jnorms	modulus for printing s.p. norms and ionization probabilities	
jcharges	modulus for printing radially averaged charge distribution	
drcharges	radial distance for scanning radially averaged charge distribution	
jplotdensitydiff	modulus for printing $\rho(t) - \rho(0)$ along x-axis	
jplotdensitydiff2d	modulus for printing 2D cuts of $\rho(t) - \rho(0)$	
jplotdensity2d	modulus for printing 2D cuts of density	
jstboostinv	modulus for evaluating boost-invariant s.p. energy and variance ???	

Namelist DYNAMIC		in for005.<name>
<i>yet unsorted</i>		
phi	phase of laser pulse, inactive for electrons, strange for ions ???	
projcharge	charge of ionic projectile	
projvelx	x-velocity of ionic point-charge projectile	
projvely	y-velocity of ionic point-charge projectile	
projvelz	z-velocity of ionic point-charge projectile	
projinix	initial x-coordinate of ionic point-charge projectile	
projiniy	initial y-coordinate of ionic point-charge projectile	
projiniz	initial z-coordinate of ionic point-charge projectile	
modionstep	modulus for ion step (nr. of electron steps per ion step)	
ispidi	=1 switches to initialization by spin-dipole boost	
mxforce	=1 zeroes forces in x-direction for nonlocal PsP ???	
myforce	=1 zeroes forces in y-direction for nonlocal PsP ???	
mzforce	=1 zeroes forces in z-direction for nonlocal PsP ???	
izforcecorr	=1 enforce zero-force condition, =0 tests condition, =-1 disables all	
dinmargin	margin defining inner box in connection with Gaussian pseudo-densities check default	
iangabso	option for origin for angular distribution (1=box, 2=c.m.)	
ipes	activates preparation of measuring points for PES	
nangtheta	number of PAD angular cones in θ direction	
nangphi	number of PAD angular cones in ϕ direction	
delomega	space angle of angular cones in PES check	
angthetal	lower angle θ for PES evaluation	
angthetah	upper angle θ for PES evaluation	
angphil	lower angle ϕ for PES evaluation	
angphihi	upper angle ϕ for PES evaluation	
ifreezekspot	=1 freezes KS potential at stage of time=0	
ifixcmion	switch to fix c.m. during ionic motion	
ekin0pp	kinetic energy for initial boost of electrons <u>and</u> ions	
vx0	boost velocity x-direction relative to ekin0pp	
vyn0	boost velocity y-direction relative to ekin0pp	
vzn0	boost velocity z-direction relative to ekin0pp	
nmptheta	number of PES measuring points in θ direction	
nmpphi	number of PES measuring points in ϕ direction	

Namelist DYNAMIC		in for005.<name>
<i>RTA parameters</i>		
jrtaint	modulus for invoking RTAS step	
rtamu	μ parameter for quadratic term on ρ -constraint	
rtamuj	μ_j parameter for quadratic term on \mathbf{j} -constraint	
rtasumvar2max	criterion for maximal variance of s.p. energies	
rtaeps	step size in DCMF iteration	
rtae0dmp	damping energy in DCMF iteration	
rtatempinit	initial temperature in RTA step	
rtaforcetemperature	is that really used?	
rtasigee	effective electron-electron cross section in RTA	
rtars	effective Wigner-Seitz radius for estimating damping rate	
Namelist EXTENSIONS		in for005.<name>
<i>extended options (not to appear in public version)</i>		
trequest	variable checking CPU time to trigger save operations	
timefrac	variable checking CPU time to trigger save operations	
iscatterelectron	switch to scattering with electron wavepacket	
jattach	modulus to compute attachment probability	
scatterelectronenergy	kinetic energy of impinging electron wavepacket	
scatterelectronvx	x-velocity of electron wavepacket (relative to energy)	
scatterelectronvyn	y-velocity of electron wavepacket (relative to energy)	
scatterelectronvzn	z-velocity of electron wavepacket (relative to energy)	
scatterelectronx	initial x-coordinate of impinging electron	
scatterelectrony	initial y-coordinate of impinging electron	
scatterelectronz	initial z-coordinate of impinging electron	
scatterelectronw	initial width of impinging electron	
jescmask	modulus for detailed print of lost electrons	
jescmaskorb	modulus for state-wise detailed print of lost electrons	
epro	energy of incoming projectile (= last ion in the list)	
vp _x , vp _y , vp _z	direction of the incoming projectile	
taccel	time span over which the projectile is accelerated to eproj for taccel=0 one has to use init_lcao=1	
nproj	element number of atomic projectile	
nproj_states	nr. of electronic states in atomic projectile	
idenspl	modulus for printing 2D cuts of density in MTV format	
i3dz	print z-integrated 2D density, following idenspl	
i3dx	print x-integrated 2D density, following idenspl	
i3dstate	print x- and z-integrated density per state, following idenspl	

	Namelist SURFACE	in for005.<name>
idielec	switch to dielectric background	
xdielec	distance of dielectric background to lowest GSM layer	
epsdi	dielectric constant of dielectric background	
isurf	switch to activate dielectric background	
ne	Number of fixed shells in substrate	
nc	number of O cores in MgO(001)	
nk	number of Mg cations in MgO(001)	
ivdw	handling of Van-der-Waals with substrate atoms 0 \Rightarrow no VdW 1 \Rightarrow enables full computation of VdW 2 \Rightarrow enables effective VdW through PsP parameters	
ifadiadip	switch to adiabatic treatment of substrate dipoles	
shiftx	global shift in x for all substrate atoms	
shifty,shiftz	as shiftx for y and z direction	
mion	mass of surface anion (16 for O in MgO(001))	
mkat	mass of surface kation (24.3 for Mg in MgO(001))	
me	mass of valence shell	
cspr	spring constant for interaction between core and valence shell	
chgc0	charge of (anion) core	
chge0	charge of valence shell	
chgk0	charge of cation	
sigmak	gauss width of cation	
sigmac	gauss width of core	
sigmav	gauss width of valence shell	
iUseCell	switch for reading/building lattice of substrate atoms 0 \Rightarrow lattice atoms are read in from input file 'for005surf.*' 1 \Rightarrow lattice is built from replicating unit cell and lattice parameters rlattvec ... are read in (see md.F)	
iPotFixed	switch for Madelung summation of substrate atoms read/write electrostatic potential from particles with imob =0, so that their run-time calculation can be skipped 0 \Rightarrow do not read; calculate full potential at each iteration 1 \Rightarrow read in potFixedIon() from previously prepared file -1 \Rightarrow calculate potFixedIon() write result to a file which can be later read in by option 1, stop after that 2 \Rightarrow calculate potFixedIon() at the beginning, do not write	
ifmdshort	includes short range interaction electron-substrate	
isrtyp(i,j)	type of interaction between the different kinds of particles 0 \rightarrow no short range interaction 1 \rightarrow GSM core 2 \rightarrow GSM valence shell =1 \Rightarrow Born-Mayer type 3 \rightarrow GSM kation =2 \Rightarrow Argon case 4 \rightarrow Na core 5 \rightarrow DFT electron	
unfixCLateralRadx	radius of cylinder with mobile cores	
unfixELateralRadx	radius of cylinder with mobile valence electrons	
fixCBelowx	fixes cores which lay below given x value	

	Namelist PERIO	in for005.<name>
ch	effective charge of ion	
amu	mass of ion in units of hydrogen mass	
dr1,dr2	radii of soft local PsP	
prho1,prho2	strenghts of soft local PsP	
crloc	radius for local part of Goedecker PsP	
cc1,cc2	strengths for local part of Goedecker PsP	
r0g,r1g,r2g	radii for non-local parts of Goedecker PsP	
h0_11g,h0_22g,h0_33g	strenghts for non-local parts of Goedecker PsP	
h1_11g,h1_22g,h2_11g	strenghts for non-local parts of Goedecker PsP	
radiong	carrier radius for projecteor in non-local Goedecker PsP	

	Namelist FSIC	in for005.<name>
step	step size in iteration of localizing or symmetry condition	
precis	precision in iteration of localizing or symmetry condition	
SymUtBegin	nr. iteration where symmetry condition starts for pure localizing step set SymUtBegin > ismax	
radmaxsym	limiting value in radius division for actual step	

	Ionic structure and e^- -initialization in for005ion.<name>
	This initialization does not use NAMELIST but reads input in fixed order. Each line stands for one ion. Each column has a definite meaning.
Col. 1	x -coordinate
Col. 2	y -coordinate
Col. 3	z -coordinate
Col. 4	number of element in periodic system (e.g.: Na \leftrightarrow 11)
Col. 5	only init_lcao=1 : ordering of nodes in repeated initialization at this ion
Col. 6	only init_lcao=1 : radius of initial Gaussian at this ion
Col. 7	only init_lcao=1 : starting spin for initalization at this ion

The handling of the initialization of electronic wavefunctions is rather involved. A more detailed explanation is given in appendix A.

A On the initialization of the electronic wavefunctions

The basic switch is `init_lcao`. The case `init_lcao=0` is the simpler option. This initializes harmonic oscillator wavefunctions about one common center. This center is usually the origin of the coordinate-space grid. It can be moved deliberately by `shiftWFx`, `shiftWFy`, and `shiftWFz`. The initial oscillator may be deformed. Its deformation is given by the dimensionless quadrupole `b2occ` and triaxiality `gamocc` (in degree). The oscillator states are filled in order of increasing oscillator energies. A spin asymmetry can be enforced with `ispinsep=1`. This option is useful when dealing with odd electron number. The upper end of initialization is determined by `deocc`. A `deocc` ≈ 0 typically initializes just as many states as are occupied. If more is required, enhance `deocc`.

The case `init_lcao=1` initializes wavefunctions which are localized at the ions. This option is richer and a bit hard to handle. In a first step, the total number of wavefunctions is estimated and it is computed how many wavefunctions have to be initialized then for each ion. At one given ion, initialization starts with the $1s$ oscillator state. The first choice of spin is taken from column 7 of `for005ion.<name>` which initializes the entry of the actual ion in the `ipol` array. The value `ipol=+1` sets a spin up (i.e. `ispin=1` in the code) as the first choice, while `ipol=-1` sets a spin down (i.e. `ispin=2`). If more than one state is to be occupied, the next is then the $1s$ state with opposite spin. Next comes the $1p_i$ state with first spin where i is the direction given as first entry in column 5. For example if column 5 selects '`yzx`', the $1p_y$ comes here. Occupation continues in order given by column 5 and 7 until the wanted number of orbitals at this ion site is reached. Column 6 sets the oscillator radius for the initialization at this ion (which allows to deal efficiently with systems consisting of very different ions). Column 7 becomes important for ions associated with an odd number of electrons as, e.g., hydrogen. One ought to distribute an equal collection of spins up and down over the whole system to avoid unnaturally polarized molecules.