

Essential Dacapo

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Minimal headers	from Dacapo import Dacapo from ASE import Atom, ListOfAtoms	
Geometry setup		
atomic positions	ListOfAtoms()	a=ListOfAtoms([(Atom('El', (x, y, z)), ...],periodic=True) (x,y,z) internal coordinates; El- chemical symbol
reading old configuration	ReadAtoms()	a = Dacapo.ReadAtoms('file')
unit cell	SetUnitCell()	a.SetUnitCell(a,b,c,)
magnetic moment	SetSpinPolarized()	a.SetSpins((1,1))
Accessing atomic properties	GetCartesianPositions()	a[1].GetCartesianPosition()
	GetKineticEnergies()	
setting up calculations	SetCalculator()	calc = Dacapo(atoms=a) a.SetCalculator(calc) a.GetPotentialEnergy()
Charge related stuff		
correction for a dipole moment in slab calculations	DipoleCorrection()	calc.DipoleCorrection(mixingparameter=0.2,initialvalue=0.0)
Electrostatic decoupling in 3D	SetElectrostaticDecoupling()	calc.SetElectrostaticDecoupling(numberofgaussians=3,ecutoff=100)
extra dipole for slab	ExternalDipolePotential()	
extra charge	ExtraCharge()	
IO control		
Naming files	SetNetCDFFile()	calc.SetNetCDFFile('test.nc')
	SetTxtFile()	calc.SetTxtFile('test.txt')
details to be saved	PrintElectronicWorkfunction()	
	CalculateAtomicDOS()	
	PrintAtomProjectedDOS()	
Geometry optimization		
atomic relaxation	Dynamics	dyn = ConjugateGradient(a,
external provided	ConjugateGradient(...)	fmax=number,lineMin=LM1(number))
by ASE	Converge()	default: number=0.05 dyn.Converge()
	SetSymmetryOff()	
unit cell stresses	CalculateStress()	calc.CalculateStress(True)
Electronic structure		
Basic setup	SetPlaneWaveCutoff()	calc.SetPlaneWaveCutoff(340)
	SetNumberOfBands()	calc.SetNumberOfBands(N) NO DEFAULT
XC functional	SetXCFunctional(exc)	calc.SetXCFunctional('PW91')
		also: 'VWN', 'PBE', 'RPBE'
k sampling	SetBZKPoints(kpts)	calc.SetBZKPoints(8,8,8)
		MonkhorstPack and ChadiCohen
efficiency	SetPseudoPotential(PSP)	calc.SetOccupationStatistics('MethfesselPaxton')
		default: 'FermiDirac'
	SetElectronicTemperature(temp)	default: temp=0.2 eV [kT]
	SetChargeMixing()	calc.SetChargeMixing(True)
		default: False
		calc.SetKerkerPreconditioning(True)
		default: False
		calc.SetEigenvalueSolver('rmm-diis')
		default: 'eigsolve'
	SetSpinPolarized()	calc.SetSpinPolarized(True)