Hartree-Fock geometry optimisation of periodic systems with the CRYSTAL code

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Supplementary material

NOTES ON THE INITIAL GEOMETRY

Table 1: Input decks. Filename and bibliographic references of the starting geometry for the periodic systems adopted as test cases.

Dim	System	Input deck	Reference
1D	Infinite water chain	polyh2o.d12	[1]
	Polyglycine	polygly.d12	[2]
	Polytetrafluoroethylene	ptfe.d12	[3]
2D	α-Al_2O_3 slab (6 atomic layers)	corun_slab.d12	[4]
	α-Cr_2O_3 slab (6 atomic layers)	acr2o3_slab.d12	[5]
	MgO(001)/CO (3 atomic layers)	mgoco.d12	[6]
3D	α-Al_2O_3	corun.d12	[4]
	α-Cr_2O_3	acr2o3.d12	[5]
	α-Quartz	quartz.d12	[7]
	α-Boron	boron.d12	[8]
	C@Si (32 atoms super-cell)	c@si.d12	[9]
	Ferroelectric ordered ice (Ice XI)	ice.d12	[10]
	α-Oxalic acid dihydrate crystal	oxa.d12	[11]
	Urea crystal	urea.d12	[12]
	Silica sodalite SOD(Si)	sodsi.d12	[13]
	Silica faujasite FAU(Si)	fausi.d12	[13]
	Titano chabazite Ti-CHA(1:1) Si:Al=1:1	ticha.d12	[14]
	Acidic chabazite H-CHA(3:1) Si:Al=3:1	hcha31.d12	[15]
	H-CHA(3:1)/NH_3	hcha31nh3.d12	[16]

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