Possible list of materials for MSE-light dataset.

The materials followed by "?" are the first to be dropped, I think, for a lighter version of MSE-light

1-d periodic
LiH

2-d periodic
LiH, C(graphene), BN, AlN?, BP?, SiC?

3-d one-element

Rare-gas fcc:	He?(hcp), Ne, Ar
bcc	Li, Na
fcc	Al
hcp	H?, Be, N?, Mg
Diamond	C (also graphite), Si
Rhombohedral	B
Orthorhombic	S,Cl
Monoclinic	O?, F
Triclinic	P?

3-d octet binaries

Rocksalt	**LiH**, **LiF**, **LiCl**, **NaF**, **NaCl**, **MgO**, **MgS**, *AlN*
Zincblende	**BeS**, **BP, AlP**, *BN*, *LiF, LiCl, MgS, BeO, AlN, SiC*
Wurtzite	**BeO**, **AlN**, **SiC**, *LiF, LiCl, MgS, BeS, BN, BP, AlP*
Graphite	**BN**

Note, in *italic* are the materials for which – according to my LDA calculations – also another crystal structure is close in energy, namely within 0.1 eV/atom. In bold are the material in their most stable phase, according to LDA (without ZPE). So, there are 13 different octet binaries, but some of them could/should be calculated in more than one crystal structure. Of course the final word (or, at least, a better guess) about relative stability needs ZPE. Should we consider it?

Basis sets
(Converged) NAO (FHI-aims-2009) and VCC-NAO-nZ

Functionals
Lattice constant(s) optimized at all levels?
LDA,
PBE,
PBE+vdW (both TS and MBD@rsSCS),
HSE06 (how many / which (α,ω)?),
HSE06+vdW (both TS and MBD@rsSCS),
XYG3 (includes B3LYP, but with geometry @ XYG3)
rPT2@PBE (includes cRPA, cRPA+rSE)
rPT2@HSE06 (includes cRPA, cRPA+rSE)
MP2@HF (includes HF)
Note: for *XYG3* and *MP2@HF* we do not have currently a periodic version implemented. If we want to have these two methods, then some slow-down is expected in order to implement the needful.

(see also page 2)

Quantities

This selection of properties is for the paper, on the website there will be more (e.g., band structure)

Cohesion energy

Equilibrium lattice constant

Bulk modulus (and B'). Note: for non-cubic systems, which EoS for B and B' ?

Band gap @ Γ (and other high symmetry points, e.g. X,L for cubic lattices)

Minimum band gap (CBm - VBM)