Computational Materials Physics

Center for Molecular Modeling

Department of Materials Science and Engineering

geometry optimization 2 : unit cell shape

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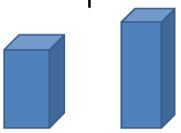
http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

only for a few high-symmetry crystals,
the volume fully determines the unit cell.

In most cases, many different unit cell shapes are possible for a given volume :

a	ℓ	0.9ℓ
b	ℓ	0.9ℓ
c	2ℓ	2.47ℓ
V	$2\ell^3$	$2\ell^3$



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6 parameters (a, b, c, α, β, γ) with one constraint (volume) = 5 degrees of freedom.

For every volume: minimize energy according to these 5 degrees of freedom

(alternative: stress tensor formalism – see later)

Can be cumbersome for low-symmetry crystals….

Doable and relevant example: hcp-Mg

- start from an experimental cif file
- vary the volume in 5 steps (±6%, ±3%, 0%)
- for every volume, vary the c/a ratio in 5 steps (±4%, ±2%, 0%)
- determine the best c/a (and corresponding energy) for every volume
- make a Birch-Murnaghan fit through the resulting 5 E(V)-points.