TremoloX - Feature #368
Hessian for Pair Potentials

09/11/2014 10:43 am - Jan Hamaekers

Status:	New		**Start date:**	09/11/2014
Priority:	Normal		**Due date:**	
Assignee:	Christian Neuen		**% Done:**	0%
Category:			**Estimated time:**	0.00 hour
Target version:				
Resolution:				

Description

Compute Hessian for all Pair potentials

(For Pascal ?)

History

#1 - 09/11/2014 10:44 am - Jan Hamaekers

- Tracker changed from Bug to Feature

#2 - 10/10/2014 09:35 am - Jan Hamaekers

- File Dave_Powell_Thesis_Final_October2006.pdf added

- File 1003.2236.pdf added

Some References to the Dynamical Matrix

We need the Hessian (which should be the "Force Constant Matrix"), which is in case of short range potentials, a sparse matrix

In a first step we should restrict us to all short range pair potentials ...

See in Powell Thesis, e.g. Chapter 5 and Appendix

See also GULP Manual 3.4.
http://nf.nci.org.au/facilities/software/Gulp/3.4/Docs/gulp3.4_manual.pdf
section 1.3.15.11 Phonons

or GULP Manual 4.2.
https://nanochemistry.curtin.edu.au/local/docs/gulp/gulp4.2_manual.pdf
1.4.16.12 Phonons

or LAMMPS
http://lammps.sandia.gov/doc/fix_phonon.html

#3 - 10/10/2014 11:16 am - Jan Hamaekers

- File 1107.0196.pdf added

See in particular
1107.0196.pdf
equation 2

#4 - 11/17/2014 09:29 am - Jan Hamaekers

- File PhysRevB.83.134118-accepted.pdf added

Should be also extended to the EAM potential

#5 - 11/17/2014 09:30 am - Jan Hamaekers

@Pascal: Can you shortly comment on the data structure you are using for the dynamical matrix, please ...

#6 - 11/17/2014 09:38 am - Jan Hamaekers

- File sfn201112007.pdf added

Refernce [41] in Shen EAM

#7 - 11/19/2014 02:58 pm - Jan Hamaekers

- File a606455h.pdf added
- File gulp4.2_manual.pdf added

see also gulp papers and manuals

Files

Dave_Powell_Thesis_Final_October2006.pdf	3 MB	10/10/2014	Jan Hamaekers
1003.2236.pdf	266 KB	10/10/2014	Jan Hamaekers
1107.0196.pdf	561 KB	10/10/2014	Jan Hamaekers
PhysRevB.83.134118-accepted.pdf	897 KB	11/17/2014	Jan Hamaekers
sfn201112007.pdf	1.66 MB	11/17/2014	Jan Hamaekers
a606455h.pdf	385 KB	11/19/2014	Jan Hamaekers
gulp4.2_manual.pdf	1.78 MB	11/19/2014	Jan Hamaekers