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Latt*E* 1.2β

first-principles lattice energy calculations

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Abstract

Latt*E* is a computer program for automatization of first-principles crystal lattice energy calculations proposed by Tsuzuki *et al.* in 2010 [1, 2]. Program consists of two parts. First part allows to prepare GJF or COM Gaussian⟨1⟩ files from crystal structure CIF file. Second part reads LOG or OUT files generated by Gaussian and perform appropriate calculations to obtain energy of crystal lattice. So on program works fine only for crystal structures with one whole molecule in asymmetric part.

1 Manual

Latt*E* is written in Java and developed as JAR files, so you need Java Runtime Environment⟨2⟩ to be installed prior to launch it. Most recent version of the program can be downloaded from its home page⟨3⟩.

If you are Microsoft Windows user you have to just double-click on JAR file to launch Latt*E*. If you are using Linux Ubuntu you have to set JAR file as executable. Right-click on JAR file, choose *Properties*, then go to *Permissions* and check the box *Allow to execute file as program*. Also ensure that in *Open with* tab Java Runtime Environment is selected. When you accept changes you can open Latt*E* just by double-clicking on JAR file.

Program window consists of two tabs (one for preparing Gaussain files and second for making final calculations) and text output box at the bottom.

⟨1⟩ www.gaussian.com
⟨2⟩ www.java.com/download
⟨3⟩ www.kchn.pg.gda.pl/latte

1.1 Prepare Gaussian files

If you have a CIF file with a crystal structure you can use it. Other files have to be converted[4]. CIF is open format file, so data reading errors can happen. Any explanation regarding data reading errors will be displayed in output box. If you cannot find a solution please contact the author.

After you put a path to CIF file you should specify radius of contact (R_{max}). This is the maximum distance between two closest atoms of two separate molecules which are taken into account (R_{min}).

Next, you should enter keywords for single molecules, dimers and periodic calculations that Gaussian will perform. Some default values are set, but feel free to modify them. By default DFT and MP2 calculations for single molecules and pairs will be performed with `B3LYP/6-31+G` and `MP2/6-31+G` method respectively. Periodic calculation will be performed with `B3LYP/3-21G*`. `%nproc`, `%mem` and `#maxdisk` inform Gaussian about amount of processors, memory and disc space to use. If your Gaussian works under Linux you should choose COM files as output format (UNIX type end-of-line). Under Windows GJF format will be fine.

After you confirm selected options Latt*E* will do its job. Cluster of molecules in specified radius is generated and then all pairs with central molecule are saved into separate files with `_001` (and so on) ending. Whole content of crystal unit cell with translation vectors is saved in file with `_cry` ending and single molecule in file with `_mol` ending. You will find all output files in the same directory where input CIF file was placed.

1.2 Make calculations in Gaussian

You should send all generated files to Gaussian. When all calculations are done then you could proceed to next step.

1.3 Calculate lattice energy

On the second tab of Latt*E* you should specify paths to all output files generated by Gaussian (OUT or LOG). After you choose type of files that Gaussian has generated you can click on Browse buttons to find appropriate files. When you open the first file and all other output files are placed in the same folder, then Latt*E* will try to add this files automatically. If not, then click other Browse buttons to select paths to the other files. In case of DFT and MP2 pairs you should specify the path to the file with `_001` ending only. Other files will be added automatically.

Additionally you can limit intermolecular distance using the cutoff option. If you set cutoff to 0 then all pairs will be considered, otherwise Latt*E* will take ony pairs with $R_{min} <$ cutoff.

When everything is set up, then you should click Calculate button at the bottom. Latt*E* will perform calculations gathering data from supplied files according to the algorithm of first principles lattice energy calculation proposed by Tsuzuki *et al.* [1].

DFT lattice energy based on difference between a whole crystal and a single molecule energy is calculated and displayed first. Then all correction terms are calculated and displayed with corresponding shortest distance between two molecules (R_{min}). Sum of these values and corrected energy is finally calculated and displayed.

[4] openbabel.org

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[1] S. Tsuzuki, H. Orita, K. Honda, M. Mikami, *J. Phys. Chem. B* **114** (2010) 6799.

[2] S. Tsuzuki, H. Orita, H. Ueki, V. A. Soloshonok, *J. Fluor. Chem.* **131** (2010) 461.