ElaStic License

August 19, 2014

ElaStic was developed by Rostam Golesorkhtabar, Jürgen Spitaler, Pasquale Pavone and Claudia Draxl in the framework of the following research projects:

- "Martensite Fundamentals and Constitutive Equations" in the framework of the Competence Centre for Excellent Technologies (COMET) on Integrated Research in Materials, Processing and Product Engineering (MPPE), with financial support by the Austrian Federal Government and the Styrian Provincial Government.
- "AtoMat Atomistic Approaches towards Materials Design" in the framework of the program line "FIT-IT Initiativen" of the program "Forschung, Innovation und Technologie für Informationstechnologien" (1. Call ModSim); Project number 819319.

ElaStic is free software and can be redistributed and/or modified under the terms of the GNU Lesser General Public License as published by the Free Software Foundation, either version 3 of the License, or (optionally) any later version. **ElaStic** is distributed without any warranty. See the GNU Lesser General Public License for more details.

Citation Requirements:

Publishing results based on **ElaStic** requires citation of the following article:

[Ref] R. Golesorkhtabar, P. Pavone, J. Spitaler, P. Puschnig, C. Draxl **ElaStic**: A tool for calculating second-order elastic constants from first principles, Computer Physics Communications 184, 1861-1873 (2013).

Also for any grant applications or patents that use **ElaStic** it must be stated that **ElaStic** was used, with a sentence such as "We used the open-source software **ElaStic** [Ref] to compute..."

Contact Info:

Jürgen Spitaler Materials Center Leoben Forschung GmbH Roseggerstraße 12, 8700 Leoben, Austria E-Mail: juergen.spitaler@mcl.at

Pasquale Pavone Humboldt-Universität zu Berlin, Solid-State Theory Group (SOL), Physics Department Zum Großen Windkanal 6, 12489 Berlin

E-Mail: pas.pav@gmail.com

1 License Information

The source header below must be included in any modification or extension of the source code of **ElaStic**.

Source Header of ElaStic:

ElaStic Version 1.0

Copyright (C) R. Golesorkhtabar, P. Pavone, J. Spitaler and C. Draxl

ElaStic is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.

ElaStic is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU Lesser General Public License for more details.

You should have received a copy of the GNU Lesser General Public License along with this program; if not, see: http://www.gnu.org/licenses/.

There are additional restrictions imposed on the use and distribution of this open-source code, including: (A) this header must be included in any modification or extension of the code; (B) you are required to cite the following paper in any publications that uses this code:

R. Golesorkhtabar, P. Pavone, J. Spitaler, P. Puschnig and C. Draxl, "ElaStic: A tool for calculating second-order elastic constants fromfirst principles", Computer Physics Communications 184, 1861-1873 (2013).