Citations

Contents

We recommend citing the original references describing the theoretical methods used when reporting results obtained from one of the *Engines* or any other module in *MedeA*, as well as giving the citation for the program itself.

Below, you can find how to cite *MedeA* and included modules appropriately. If you have any questions, please forward these to support@materialsdesign.com.

1 *MedeA* Environment

MedeA 3.10; *MedeA* is a registered trademark of Materials Design, Inc., San Diego, USA.

2 Engines

2.1 VASP

The calculations have been performed with *MedeA VASP* using the ab-initio total-energy and molecular-dynamics package VASP (Vienna ab-initio simulation package) developed at the Institut für Materialphysik of the Universität Wien [1,2].

[1] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11169 (1996).

[2] G. Kresse and J. Furthmüller, Comput. Mat. Sci. **6**, 15 (1996).

If the PAW potentials are used, in addition reference need to be to:

[3] G. Kresse and D. Joubert, Phys. Rev. B **59**, 1758 (1999).

If special features implemented in VASP have been used, reference should be made to the relevant publications as listed on the VASP website.

2.2 GIBBS

The calculations have been performed with *MedeA GIBBS* , using: Gibbs 9.7.8, IFP Energies Nouvelles, Rueil-Malmaison & Laboratoire de Chimie-Physique, Université Paris Sud, CNRS, France [1-5].

[1] P. Ungerer, C. Beauvais, J. Delhommelle, A. Boutin, B. Rousseau, and A. H. Fuchs, J. Chem. Phys. **112**, 5499-5510 (2000).

[2] E. Bourasseau, M. Haboudou, A. Boutin, A. H. Fuchs, and P. Ungerer, J. Chem. Phys. **118**, 3020-3034 (2003).

[3] A. D. Mackie, B. Tavitian, A. Boutin, and A. H. Fuchs, Mol. Simul. **19**, 1-15 (1997).

[4] M. Lagache, P. Ungerer, A. Boutin, and A. H. Fuchs, Phys. Chem. Chem. Phys. **3**, 4333-4339 (2001).

[5] E. Bourasseau, P. Ungerer, A. Boutin, and A. H. Fuchs, Mol. Simul. **28**, 317-336 (2002).

[6] N. Ferrando, A. Boutin, and V. Lachet, J. Phys. Chem. **114**, 8680-8688 (2010).

2.3 LAMMPS

The calculations have been performed with *MedeA LAMMPS* , using: LAMMPS 17-Apr-2024. LAMMPS stands for Large-scale Atomic/Molecular Massively Parallel Simulator.

The following CPC paper [1] is the canonical reference to use for citing LAMMPS. It gives an overview of the code including its parallel algorithms, design features, performance, and brief highlights of many of its materials modeling capabilities. If you wish, you can also mention the URL of the LAMMPS website in your paper, namely https://www.lammps.org.

[1] A. P. Thompson, H. M. Aktulga, R. Berger, D. S. Bolintineanu, W. M. Brown, P. S. Crozier, P. J. in 't Veld, A. Kohlmeyer, S. G. Moore, T. D. Nguyen, R. Shan, M. J. Stevens, J. Tranchida, C. Trott, and S. J. Plimpton, Comp. Phys. Comm. **271**, 10817 (2022).

This earlier JCP paper [2] was the original citation for LAMMPS. You can cite it if you want to refer to the parallel spatial-decomposition strategy LAMMPS still uses:

[2] S. Plimpton, J. Comp. Phys. **117**, 1-19 (1995).

If special features implemented in LAMMPS have been used, reference should be made to the relevant publications as listed on the LAMMPS website https://www.lammps.org/cite.html.

2.4 Gaussian

The calculations have been performed with *MedeA Gaussian* , using: Gaussian 16

For proper citation of Gaussian 16, see https://gaussian.com/citation/

2.5 MOPAC

The calculations have been performed with *MedeA MOPAC* , using: MOPAC2016 17.048 [1]

[1] James J. P. Stewart, Stewart Computational Chemistry, Colorado Springs, CO, USA, http://OpenMOPAC.net (2016).

3 *InfoMaticA* & Databases

MedeA InfoMaticA version *1.0*

3.1 *ICSD*

3.2 *Pearson*

3.3 *NIST*

4 Property Modules

4.1 *MT*

The calculations have been performed with *MedeA MT*. The symmetry-general methodology employed by *MedeA MT* is described in:

[1] Y. Le Page and P. W. Saxe, Phys. Rev. B **63**, 174103 (2001).

[2] Y. Le Page and P. W. Saxe, Phys. Rev. B **65**, 104104 (2002).

When sampling sets of structures, *MedeA MT* employs the Hill-Walpole method, as described in:

[3] U. W. Suter and B. E. Eichinger, Polymer **43**, 575 (2002).

4.2 Phonon

The calculations have been performed with *MedeA Phonon* using: PHONON Software 6.14, Copyright © Prof. Krzysztof PARLINSKI [1].

[1] K. Parlinski, Z. Q. Li, and Y. Kawazoe, Phys. Rev. Lett. **78**, 4063 (1997).

4.3 *Transition State Search*

The calculations have been performed with *MedeA Transition State Search*.

4.4 *Electronics*

The calculations have been performed with *MedeA Electronics*.

If transport functions are calculated, reference should be made to the Boltzmann Transport Properties (BoltzTraP) code version 1.2.2 [1].

[1] G. K. H. Madsen and D. J. Singh, Comput. Phys. Commun. **175**, 67 (2006)

4.5 *MLPG*

If a Neural Network Potential has been generated please cite as follows:

The calculations have been performed with *MedeA MLPG*, using a Neural Network Potential (NNP) as generated by the n2p2 code [1], [2] with symmetry functions defined in [3], [4], and [5].

[1] A. Singraber, J. Behler, and C. Dellago, Library-Based LAMMPS Implementation of High-Dimensional Neural Network Potentials. J. Chem. Theory Comput. 15, 1827-1840 (2019) (https://doi.org/10.1021/acs.jctc.8b00770)

[2] A. Singraber, T. Morawietz, J. Behler, and C. Dellago, Parallel Multistream Training of High-Dimensional Neural Network Potentials. J. Chem. Theory Comput. 15, 3075-3092 (2019) (https://doi.org/10.1021/acs.jctc.8b01092)

[3] J. Behler and M. Parrinello, Phys. Rev. Lett. 98, 146401 (2007)

[4] G. Imbalzano et al., J. Chem. Phys. 148, 241730 (2018)

[5] M. Gastegger et al., J. Chem. Phys. 148, 241709 (2018)

In contrast, if a Spectral Neighbor Analysis POtential has been generated please cite as follows:

The calculations have been performed with *MedeA MLPG*, using a Spectral Neighbor Analysis Potential (SNAP) as generated by the FitSNAP code [1], [2], and [3].

[1] A. P. Thompson, L. P. Swiler, C. R. Trott, S. M. Foiles, and G. J. Tucker, Spectral neighbor analysis method for automated generation of quantum-accurate interatomic potentials, J. Comp. Phys. 285, 316-330 (2015) (https://doi.org/10.1016/j.jcp.2014.12.018)

[2] M. A. Wood and A. P. Thompson, Extending the accuracy of the SNAP interatomic potential form, J. Chem. Phys. 148, 241721 (2018) (https://doi.org/10.1063/1.5017641)

[3] M. A. Cusentino, M. A. Wood, and A. P. Thompson, Explicit Multielement Extension of the Spectral Neighbor Analysis Potential for Chemically Complex Systems, J. Phys. Chem. A 124, 5456-5464 (2020) (https://doi.org/10.1021/acs.jpca.0c02450)

4.6 UNCLE

The calculations have been performed with *MedeA UNCLE*, using the UNiversal CLuster Expansion (UNCLE) code [1].

[1] D. Lerch, O. Wieckhorst, G. L. W. Hart, R.W. Forcade, and S. Müller, "UNCLE: a code for constructing cluster expansions for arbitrary lattices with minimal user-input", Modelling Simul. Mater. Sci. Eng. **17**, 055003 (2009).

4.7 *P3C*

The calculations have been performed with *MedeA P3C*, using Correlations as those developed by J. Bicerano [1].

[1] Prediction of Polymer Properties (Third Edition), Jozef Bicerano, Marcel Dekker, Inc., 2002

4.8 *QSPR*

The calculations have been performed with *MedeA QSPR*, using the Group Contribution method of Joback [1].

[1] K. G. Joback, R. C. Reid, *Estimation of Pure-Component Properties from Group-Contributions*, Chem. Eng. Commun. **57**, 233-243 (1987).