

8. REFERENCES

- [1] Goedecker, S. J. 2004. Minima hopping: An efficient search method for the global minimum of the potential energy surface of complex molecular systems. *J. Chem. Phys.* 120, 21, 9911-9917. DOI=10.1063/1.1724816.
- [2] Wales, D. J., and Doye, J. P. K. 1997. Global Optimization by Basin-Hopping and the Lowest Energy Structures of Lennard-Jones Clusters Containing up to 110 Atoms. *J. Phys. Chem. A* 101, 28, 5111-5116. DOI= 10.1021/jp970984n.
- [3] Call, S. T., Zubarev, D. Y., and Boldyrev, A. I. 2007. Global minimum structure searches via particle swarm optimization. *J. Comput. Chem.* 28, 7, 1177-1186. DOI= 10.1002/jcc.20621
- [4] Pickard, C. J. and Needs, R. J. 2011. Ab initio random structure searching *J. Phys.: Condens. Matter.* 23, 5, 053201. DOI=10.1088/0953-8984/23/5/053201
- [5] Hartke, B.J. 1993. Global geometry optimization of clusters using genetic algorithms. *J. Phys. Chem.* 97, 39, 9973-9976. DOI=10.1021/j100141a013
- [6] Lohn, J. D., Hornby, G. S., and Linden, D. D. 2005, An evolved antenna for deployment on NASA's Space Technology 5 Mission. In *Genetic Programming Theory and Practice II. Genetic Programming, Vol 8.* U. M. O'Reilly, T. Yu, R. Riolo, and B. Worzel Eds. Springer, Boston, MA.
- [7] Jørgensen, M. S., Groves, M. N., and Hammer, B. 2017, Combining Evolutionary Algorithms with Clustering toward Rational Global Structure Optimization at the Atomic Scale, *J. Chem. Theory Comput.* 13, 3, 1486-1493. DOI=10.1021/acs.jctc.6b01119
- [8] Turing, A. M. 1950, "Computing machinery and intelligence". *Mind.* 59, 236, 433-460. DOI=10.1093/mind/LIX.236.433
- [9] Rechenberg, I. 1973. *Evolutionsstrategie.* Holzmann-Froboog, Stuttgart.
- [10] Fogel, D. B. (editor) 1998. *Evolutionary Computation: The Fossil Record.* IEEE Press., New York, NY
- [11] Holland, J. 1992. *Adaptation in Natural and Artificial Systems.* MIT Press. Cambridge, MA.
- [12] Aldawoodi, N. 2008. *An Approach to Designing an Unmanned Helicopter Autopilot Using Genetic Algorithms and Simulated Annealing.* Doctoral Thesis. University of South Florida
- [13] Evolver: Sophisticated Optimization for Spreadsheets. 2019. Palisade. <https://www.palisade.com/evolver/>
- [14] Lyakhov A.O., Oganov A.R., and Valle M. 2010. How to predict very large and complex crystal structures. *Comp. Phys. Comm.* 181, 9, 1623-1632. DOI= 10.1016/j.cpc.2010.06.007
- [15] Vilhelmsen L. B., and Hammer, B. 2014. A genetic algorithm for first principles global structure optimization of supported nano structures. *J. Chem. Phys.* 141, 4, 044711. DOI= 10.1063/1.4886337.
- [16] Zhai, H., and Anastassia N. Alexandrova. 2017. Fluxionality of Catalytic Clusters: When It Matters and How to Address It. *ACS Catal.* 7, 3, 1905-1911. DOI= 10.1021/acscatal.6b03243
- [17] Lones, M. A., and Tyrrell, A. M. 2007. Regulatory Motif Discovery Using a Population Clustering Evolutionary Algorithm. *IEEE/ACM Transactions On Computational Biology And Bioinformatics.* 4, 3, 403-414. DOI= 10.1109/tcbb.2007.1044
- [18] Lipkowitz, K.B. and Boyd, D.B. 2003. *Reviews in Computational Chemistry, Vol. 18.* John Wiley & Sons, New York, NY.
- [19] Anderson E, Veith GD, Weininger D. 1987. SMILES: A line notation and computerized interpreter for chemical structures. U.S. EPA, Environmental Research Laboratory-Duluth. Duluth, MN
- [20] Weininger, D. 1988. SMILES, a chemical language and information system. 1. Introduction to methodology and encoding rules, *J. Chem. Inf. Comp. Sci.* 28, 1, 31-36, DOI: 10.1021/ci00057a005
- [21] Fletcher, R. 1987. *Practical methods of optimization* (2nd ed.), John Wiley & Sons, New York, NY
- [22] Elstner, M., Seifert, G. 2014, Density functional tight binding. *Phil. Trans. R. Soc. London, Ser. A.* 372. 20120483. DOI=10.1098/rsta.2012.0483
- [23] Aradi, B., Hourahine, B., and Frauenheim, 2007. Th. DFTB+, a sparse matrix-based implementation of the DFTB method, *J. Phys. Chem. A.* 111, 26, 5678-5684. DOI=10.1021/jp070186p
- [24] Larsen, A. H., Mortensen, J. J., Blomqvist, J., Castelli, I. E., Christensen, R., Dułak, M., Friis, J., Groves, M. N., Hammer, B., Hargus, C., Hermes, E. D., Jennings, P. C., Jensen, P. B., Kermode, J., Kitchin, J. R., Kolsbjerg, E. L., Kubal, J., Kaasbjerg, K., Lysgaard, S., Maronsson, J. B., Maxson, T., Olsen, T., Pastewka, L., Peterson, A., Rostgaard, C., Schiøtz, J., Schütt, O., Strange, M., Thygesen, K. S., Vegge, T., Vilhelmsen, L., Walter, M., Zeng, Z., Jacobsen, K. W. 2017. The Atomic Simulation Environment—A Python library for working with atoms, *J. Phys.: Condens. Matter.* 29, 27, 273002. DOI= 10.1088/1361-648x/aa680e