How to cite Multiwfn

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Last update: 2024-Apr-1

Multiwfn is free-of-charge and not funded. The **best way** of supporting continued development of Multiwfn is properly citing my related works.

If Multiwfn is used in your research, **citing the original paper of Multiwfn is always mandatory**:

> Tian Lu, Feiwu Chen, Multiwfn: A Multifunctional Wavefunction Analyzer, *J. Comput. Chem*. **33**, 580-592 (2012) DOI: 10.1002/jcc.22885

Whenever possible, please mention and cite Multiwfn in main text rather than in supplemental information, otherwise not only Multiwfn will be difficult for readers to notice, but also the paper will not be included in citation statistics.

Other papers should ***also*** be cited according to the method and the function employed in your work, as described below.

• Quantitative molecular surface analysis (main function 12). In below paper the algorithm of this analysis and implementation in Multiwfn were described in detail

> Tian Lu, Feiwu Chen, Quantitative analysis of molecular surface based on improved Marching Tetrahedra algorithm, *J. Mol. Graph. Model.*, **38**, 314-323 (2012) DOI: 10.1016/j.jmgm.2012.07.004

• Hole-electron analysis (subfunction 1 of main function 18)

> Zeyu Liu, Tian Lu, Qinxue Chen, An sp-hybridized all-carboatomic ring, cyclo[18]carbon: Electronic structure, electronic spectrum, and optical nonlinearity, *Carbon*, **165**, 461-467 (2020) DOI: 10.1016/j.carbon.2020.05.023

• Electrostatic potential evaluation algorithm employed by Multiwfn (Please cite this if electrostatic potential is analyzed via Multiwfn):

> Jun Zhang, Tian Lu, Efficient Evaluation of Electrostatic Potential with Computerized Optimized Code, *Phys. Chem. Chem. Phys.*, **23**, 20323-20328 (2021) DOI: 10.1039/D1CP02805G

• sobEDA and sobEDAw energy decomposition analysis

> Tian Lu, Qinxue Chen, Simple, Efficient, and Universal Energy Decomposition Analysis Method Based on Dispersion-Corrected Density Functional Theory, *J. Phys. Chem. A*, **127**, 7023-7035 (2023) DOI: 10.1021/acs.jpca.3c04374

• Orbital composition analysis (main function 8). In below paper different orbital composition calculation methods are detailedly compared and discussed

Tian Lu, Feiwu Chen, Calculation of Molecular Orbital Composition, *Acta Chim. Sinica*, **69**, 2393-2406 (2011) (in Chinese)
http://sioc-journal.cn/Jwk_hxxb/CN/abstract/abstract340458.shtml

• Charge decomposition analysis (CDA) (main function 16). In below paper the generalized CDA method (GCDA) that implemented in Multiwfn is introduced

Meng Xiao, Tian Lu, Generalized Charge Decomposition Analysis (GCDA) Method, *Journal of Advances in Physical Chemistry*, **4**, 111-124 (2015) (in Chinese) http://dx.doi.org/10.12677/JAPC.2015.44013

• Atomic dipole moment corrected Hirshfeld (ADCH):

Tian Lu, Feiwu Chen, Atomic dipole moment corrected Hirshfeld population method, *J. Theor. Comput. Chem.*, **11**, 163-183 (2012) DOI: 10.1142/S0219633612500113

• Population analysis module (main function 7). Citation is suggested but not mandatory:

Tian Lu, Feiwu Chen, Comparison of Computational Methods for Atomic Charges, *Acta Phys. -Chim. Sin.*, **28**, 1-18 (2012) (in Chinese) DOI: 10.3866/PKU.WHXB2012281

• Laplacian bond order (LBO):

Tian Lu, Feiwu Chen, Bond Order Analysis Based on the Laplacian of Electron Density in Fuzzy Overlap Space, *J. Phys. Chem. A*, **117**, 3100-3108 (2013) DOI: 10.1021/jp4010345

• Statistical analysis of area in different ESP ranges on vdW surface

Tian Lu, Sergio Manzetti, Wavefunction and reactivity study of benzo[a]pyrene diol epoxide and its enantiomeric forms, *Struct. Chem.*, **25**, 1521-1533 (2014)
DOI: 10.1007/s11224-014-0430-6

• Charge-transfer spectrum. This method was proposed by me in this paper

Zeyu Liu, Xia Wang, Tian Lu, et al., Potential optical molecular switch: Lithium@cyclo[18]carbon complex transforming between two stable configurations, *Carbon*, **187**, 78-85 (2022) DOI: 10.1016/j.carbon.2021.11.005

• Electron localization function (ELF). This paper clarified definition of ELF and explicitly derived the ELF for open-shell case, which is the form implemented in Multiwfn

Tian Lu, Feiwu Chen, Meaning and Functional Form of the Electron Localization Function, *Acta Phys. -Chim. Sin.*, **27**, 2786-2792 (2011)
DOI: 10.3866/PKU.WHXB20112786

• Analysis of valence electron and deformation density

Tian Lu, Qinxue Chen, Revealing Molecular Electronic Structure via Analysis of Valence Electron Density, *Acta Phys. -Chim. Sin.*, **34**, 503-513 (2018)
DOI: 10.3866/PKU.WHXB201709252

• Predicting binding energy of hydrogen bonds based properties of bond critical point:

> Saeedreza Emamian, Tian Lu, Holger Kruse, Hamidreza Emamian, Exploring Nature and Predicting Strength of Hydrogen Bonds: A Correlation Analysis Between Atoms-in-Molecules Descriptors, Binding Energies, and Energy Components of Symmetry-Adapted Perturbation Theory, *J. Comput. Chem.*, **40**, 2868-2881 (2019) DOI: 10.1002/jcc.26068

• π electron analysis based on localized molecular orbitals (*e.g.* subfunction 22 of main function 100):

> Tian Lu, Qinxue Chen, A simple method of identifying π orbitals for non-planar systems and a protocol of studying π electronic structure, *Theor. Chem. Acc.*, **139**, 25 (2020) DOI: 10.1007/s00214-019-2541-z

• van der Waals potential analysis (subfunction 6 of main function 20)

> Tian Lu, Qinxue Chen, van der Waals Potential: An Important Complement to Molecular Electrostatic Potential in Studying Intermolecular Interactions, *J. Mol. Model.*, **26**, 315 (2020) DOI: 10.1007/s00894-020-04577-0

• Interaction region indicator (IRI) (subfunction 4 of main function 20)

> Tian Lu, Qinxue Chen, Interaction Region Indicator (IRI): A Simple Real Space Function Clearly Revealing Both Chemical Bonds and Weak Interactions, *Chemistry-Methods*, **1**, 231 (2021) DOI: 10.1002/cmtd.202100007

• Independent gradient model based on Hirshfeld partition (IGMH) (subfunction 11 of main function 20). If you use independent gradient model (IGM), please also cite this paper along with original paper of IGM, since this paper presents a detailed overall of IGM and describes its implementation in Multiwfn.

> Tian Lu, Qinxue Chen, Independent gradient model based on Hirshfeld partition: A new method for visual study of interactions in chemical systems, *J. Comput. Chem.*, **43**, 539 (2022) DOI: 10.1002/jcc.26812
> Tian Lu, Qinxue Chen, Erratum to "Independent gradient model based on Hirshfeld partition: A new method for visual study of interactions in chemical systems", *ChemRxiv* (2022) DOI: https://doi.org/10.26434/chemrxiv-2022-g1m34

• $ICSS_{ZZ}$ map (subfunction 3 in main function 25)

> Zeyu Liu, Tian Lu, Qinxue Chen, An sp-hybridized all-carboatomic ring, cyclo[18]carbon: Bonding character, electron delocalization, and aromaticity, *Carbon*, **165**, 468-475 (2020) DOI: 10.1016/j.carbon.2020.04.099

• MO-PDOS map (Option -2 in main function 10)

> Zeyu Liu, Tian Lu, Qinxue Chen, An sp-hybridized all-carboatomic ring, cyclo[18]carbon: Electronic structure, electronic spectrum, and optical nonlinearity, *Carbon*, **165**, 461-467 (2020) DOI: 10.1016/j.carbon.2020.05.023

• Molecular polarity index (MPI) (outputted by main function 12)

> Zeyu Liu, Tian Lu, Qinxue Chen, Intermolecular interaction characteristics of the all-carboatomic ring, cyclo[18]carbon: Focusing on molecular adsorption and stacking, *Carbon*, **171**, 514-523 (2021) DOI: 10.1016/j.carbon.2020.09.048

• Analysis of valence electron and deformation density

> Tian Lu, Qinxue Chen, Revealing Molecular Electronic Structure via Analysis of Valence Electron Density, *Acta Phys. -Chim. Sin.*, **34**, 503-513 (2018)
> DOI: 10.3866/PKU.WHXB201709252

• Studying molecular planarity via MPP, SDP and coloring atoms according to d^s values

> Tian Lu, Simple, reliable, and universal metrics of molecular planarity, *J. Mol. Model.*, **27**, 263 (2021) DOI: 10.1007/s00894-021-04884-0

• Energy decomposition analysis based on force field (EDA-FF). This paper is my first public paper describing EDA-FF analysis

> Tian Lu, Zeyu Liu, Qinxue Chen, Comment on "18 and 12 – Member carbon rings (cyclo[n]carbons) – A density functional study", *Mat. Sci. Eng. B-Adv.*, **273**, 115425 (2021) DOI: 10.1016/j.mseb.2021.115425

• Conceptual density functional theory (CDFT) and information-theoretic approach (ITA) analyses. This book chapter comprehensively describes features and implementations of these functions in Multiwfn.

> Tian Lu, Qinxue Chen, Realization of Conceptual Density Functional Theory and Information-Theoretic Approach in Multiwfn Program. In *Conceptual Density Functional Theory*, WILEY-VCH GmbH: Weinheim (2022); pp 631-647. DOI: 10.1002/9783527829941.ch31

• .mwfn format. In this paper other file formats such as .fch, .wfn, .wfx, .molden are also collectively introduced

> Tian Lu, Qinxue Chen, mwfn: A Strict, Concise and Extensible Format for Electronic Wavefunction Storage and Exchange, *ChemRxiv* (2020)
> DOI: 10.26434/chemrxiv.11872524