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Knowledge Inn (in nature)

- **Research Profile of Dr. Donald Truhlar**
- **Knowledge cycle**

KLab
rsr.chem1979

Research Profile of Donald Truhlar

Donald Truhlar
University of Minnesota

Born on February 27, 1944
Chicago, US

	All	Since 2014
Citations	1,60,116	68,016
h-index	169	98
# Publications	Approx. 1,200	

Accessed on 30-09-2019

Typical titles of research output of Donald Truhlar high impact (# citations) publications		
TITLE	**# Citations**	**Year**
The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new … Y Zhao, DG Truhlar Theoretical Chemistry Accounts 120 (1-3), 215-241	**15,295**	2008
Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions AV Marenich, CJ Cramer, DG Truhlar The Journal of Physical Chemistry B 113 (18), 6378-6396	**5,896**	2009
Density functionals with broad applicability in chemistry Y Zhao, DG Truhlar Accounts of chemical research 41 (2), 157-167	**4989**	2008
A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions Y Zhao, DG Truhlar The Journal of chemical physics 125 (19), 194101	3286	2006
Design of density functionals by combining the method of constraint satisfaction with parametrization for thermochemistry, thermochemical kinetics, and noncovalent interactions Y Zhao, NE Schultz, DG Truhlar Journal of Chemical Theory and Computation 2 (2), 364-382	2840	2006
Implicit solvation models: equilibria, structure, spectra, and dynamics CJ Cramer, DG Truhlar Chemical Reviews 99 (8), 2161-2200	2364	1999
Current status of transition-state theory DG Truhlar, BC Garrett, SJ Klippenstein The Journal of physical chemistry 100 (31), 12771-12800	1617	1996
Variational transition-state theory	1579*	1980

Typical titles of research output of Donald Truhlar high impact (# citations) publications		
DG Truhlar, BC Garrett Accounts of Chemical Research 13 (12), 440-448		
Adiabatic connection for kinetics BJ Lynch, PL Fast, M Harris, DG Truhlar The Journal of Physical Chemistry A 104 (21), 4811-4815	1473	2000
Hybrid meta density functional theory methods for thermochemistry, thermochemical kinetics, and noncovalent interactions: the MPW1B95 and MPWB1K models and comparative … Y Zhao, DG Truhlar The Journal of Physical Chemistry A 108 (33), 6908-6918	1467	2004
Ab initio molecular dynamics: basic theory and advanced methods D Marx, J Hutter Cambridge University Press	1307	2009
Density functional theory for transition metals and transition metal chemistry CJ Cramer, DG Truhlar Physical Chemistry Chemical Physics 11 (46), 10757-10816	1234	2009
Chemical applications of atomic and molecular electrostatic potentials: reactivity, structure, scattering, and energetics of organic, inorganic, and biological systems P Politzer, DG Truhlar Springer Science & Business Media	1211	2013
Advances in molecular quantum chemistry contained in the Q-Chem 4 program package Y Shao, Z Gan, E Epifanovsky, ATB Gilbert, M Wormit, J Kussmann, ... Molecular Physics 113 (2), 184-215	1207	2015
How enzymes work: analysis by modern rate theory and computer simulations M Garcia-Viloca, J Gao, M Karplus, DG Truhlar Science 303 (5655), 186-195	1073	2004

Typical titles of research output of Donald Truhlar high impact (# citations) publications		
Design of density functionals that are broadly accurate for thermochemistry, thermochemical kinetics, and nonbonded interactions Y Zhao, DG Truhlar The Journal of Physical Chemistry A 109 (25), 5656-5667	998	2005
Density functional for spectroscopy: no long-range self-interaction error, good performance for Rydberg and charge-transfer states, and better performance on average than B3LYP … Y Zhao, DG Truhlar The Journal of Physical Chemistry A 110 (49), 13126-13130	987	2006
QM/MM: what have we learned, where are we, and where do we go from here? H Lin, DG Truhlar Theoretical Chemistry Accounts 117 (2), 185	974	2007
Variational transition-state theory DG Truhlar, BC Garrett Accounts of Chemical Research 13 (12), 440-448	933	1980
Exchange-correlation functional with broad accuracy for metallic and nonmetallic compounds, kinetics, and noncovalent interactions Y Zhao, NE Schultz, DG Truhlar The Journal of chemical physics 123 (16), 161103	916	2005
Variational transition state theory DG Truhlar, BC Garrett Annual Review of Physical Chemistry 35 (1), 159-189	908	1984
Benchmark databases for nonbonded interactions and their use to test density functional theory Y Zhao, DG Truhlar Journal of Chemical Theory and Computation 1 (3), 415-432	866	2005
Parametrized models of aqueous free energies of solvation based on pairwise descreening of solute atomic charges from a dielectric medium GD Hawkins, CJ Cramer, DG Truhlar The Journal of Physical Chemistry 100 (51), 19824-19839	843	1996

Typical titles of research output of Donald Truhlar high impact (# citations) publications		
On the determination of Born–Oppenheimer nuclear motion wave functions including complications due to conical intersections and identical nuclei CA Mead, DG Truhlar The Journal of Chemical Physics 70 (5), 2284-2296	836	1979
Molecular modeling of the kinetic isotope effect for the [1, 5]-sigmatropic rearrangement of cis-1, 3-pentadiene YP Liu, GC Lynch, TN Truong, DH Lu, DG Truhlar, BC Garrett Journal of the American Chemical Society 115 (6), 2408-2415	803	1993
Quantum mechanical methods for enzyme kinetics J Gao, DG Truhlar Annual Review of Physical Chemistry 53 (1), 467-505	761	2002
Current status of transition-state theory DG Truhlar, WL Hase, JT Hynes The Journal of Physical Chemistry 87 (15), 2664-2682	754	1983

Academic profile of ofDonald Truhlar			
B.A.	St. Mary's College of Minnesota	1965	
Ph. D	Caltech	1970	Doctoral advisor Aron Kuppermann
Faculty	University of Minnesota	1969–present	

Awards (to) Donald Truhlar		
Award	**for**	**year**
ACS	Theoretical Chemistry	2019
Royal Society	Chemistry Chemical Dynamics	2012
ACS Peter Debye Award	Physical Chemistry	2006
Minnesota	Outstanding contributions to chemical sciences	2003
ACS	Computers in Chemical and Pharmaceutical	2000

NSF	Research Creativity Award	1993

Donald Truhlar		
Expertise		
Developing new density functionals (Minnesota Functionals) for practical calculations		Thermochemistry Thermochemical kinetics Noncovalent interactions
Theoretical chemistry Computational chemistry Computational quantum chemistry	→	Kinetics dynamics Solvation Electronic structure Catalysis Density Functional Theory Basis sets
More accurate and more efficient		Simulations
Atmospheric Environmental chemistry;		Drug design; Nanoparticle structure Energetics Health Industrial materials
Major disciplines o Physics o Chemistry/Computation o Biology		
Synergy o Molecular simulation o Electronic structure theory o Intelligence o Machine learning o Experiment o Knowledge; Information Data (Kid)		

Knowledge* cycle (Data to Consciousness)
Evolution (Natural, Laboratory) ▪ Theory, science fiction, Philosophy, beliefs, Religion, mutated ideas

- Formal training, research, experience,
- Exploration (results known/unknown)
-
- Observation (probe: humans sense organs, instruments)
  - → Data
- Computing (human thinking, Machine computation)
  - → Information
- Research (Trained (expert) human brain)
  - → Generates knowledge
  - → Extracts knowledge
  - Extracts meta, meta …., knowledge
- Consolidation by Brain
  - Knowledge gets capsuled → intelligence
  - Intelligence, experience and all form consciousness in a niche

* Knowledge : [Experiment, Computation, Simulation]

GREATEST BENEFIT TO MANKIND

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