
ALEXANDRE TKATCHENKO

Professor, Chair of Theoretical Chemical Physics

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RESEARCH ACTIVITIES

- Electronic structure theory (density-functional theory, quantum chemistry)
- Intermolecular interactions, many-body effects in chemistry and physics
- Applications of electronic structure methods to molecules, solids, and composites
- Machine learning applied to molecules and materials

POSITIONS

2015 – present: Chair of Theoretical Chemical Physics, University of Luxembourg.

Since 2017: Distinguished visiting fellow at Berlin Big Data Center.

2011 – 2016: Group Leader and ERC Starting Grant Holder, Fritz Haber Institute, Berlin, Germany.

2012: Distinguished Visiting Professor, Pohang Institute of Science and Technology, South Korea.

2007 – 2010: Alexander von Humboldt Postdoctoral Fellow, Fritz Haber Institute, Berlin, Germany.

EDUCATION

2007: Ph.D. degree, Physical Chemistry, Universidad Autonoma Metropolitana, Mexico.

2003: B.Sc. degree, Computer Science, Universidad Autonoma Metropolitana, Mexico.

PUBLICATIONS / CONFERENCES

110 publications (h-index of 46, > 8600 citations), including Science (2), Science Advances (2), Nature Communications (5), Proc. Natl. Acad. Sci. USA (2), Phys. Rev. Lett. (22), Chem. Sci. (3), Angew. Chem., JACS (2). 6 plenary talks, 90 invited talks, 80 invited seminars/colloquia at labs and universities worldwide, more than 200 contributed talks from my group.

Relevant papers

1. A. Tkatchenko and M. Scheffler, *Accurate Molecular van der Waals Interactions From Ground-State Electron Density and Free-Atom Reference Data*, **Phys. Rev. Lett.** 102, 073005 (2009) (2050 citations, 8th most cited paper in PRL 2009–2014).
2. A. Ambrosetti, N. Ferri, R. A. DiStasio Jr., and A. Tkatchenko, *Wavelike Charge Density Fluctuations and van der Waals Interactions at the Nanoscale*, **Science** 351, 1171 (2016).
3. S. Chmiela, A. Tkatchenko, H.E. Sauceda, I. Poltavsky, K.T. Schütt, and K.-R. Müller, *Machine Learning of Accurate Energy-Conserving Molecular Force Fields*, **Science Adv.** 3, 1603015 (2017).
4. J. Hermann, D. Alfè, and A. Tkatchenko, *Nanoscale π - π stacked molecules are bound by collective charge fluctuations*, **Nature Commun.** 8, 14052 (2017).
5. J. Hermann, R.A. DiStasio Jr., and A. Tkatchenko, *First-Principles Models for van der Waals Interactions in Molecules and Materials: Concepts, Theory, and Applications*, **Chem. Rev.** 117, 4714-4758 (2017).
6. K.T. Schütt, F. Arbabzadah, S. Chmiela, K.R. Müller, and A. Tkatchenko, *Quantum-chemical insights from deep tensor neural networks*, **Nature Commun.** 8, 13890 (2017).

AWARDS

- NSF PhD Fellow (2005), NSF Senior Fellow (2011), and Program Chair (2016) at *Institute for Pure and Applied Mathematics* at University of California at Los Angeles, Los Angeles, USA.
- Research Fellowship from *Alexander von Humboldt Foundation*, Germany.
- Lindau Nobel Laureates Meeting (dedicated to Physics with 25 Nobel Laureates) at Lake Konstanz,

- Germany. Selected in a world wide competition between young scientists.
- Volker Heine Awardee at the *Psi_k 2010 Conference*.
- Gerhard Ertl Young Investigator Award at *DPG Spring Meeting*, Dresden, Germany.
- ERC Starting Grant “*VDW-CMAT*” (1.4 million Euro for 5 years) from the European Research Council, 2011-2016.
- ERC Consolidator Grant “*BeStMo*” (1.8 million Euro for 5 years) from the European Research Council, 2017-2022.
- Woodward Lecture in the Chemical Sciences (Physical Chemistry) at Harvard University.

SUPERVISIONS

9 PhDs (7 as supervisor and 2 as co-supervisor) and 14 post docs – cf appendix for details

TEACHING

March–July 2013: “Condensed Matter Physics I and II”, Technical University, Berlin.

March–July 2014: “Theory of Intermolecular Interactions”, Technical University, Berlin.

2016, 2017: “Mathematical Physics: Classical Mechanics”, University of Luxembourg.

REVIEWING – EXPERTISE – COMMITTEES - CONFERENCES

- Reviewer for 20 ISI journals (80 papers in 2016), including Nature Materials, Nature Communications, Phys. Rev. Lett., JACS, Chem. Sci., Angew. Chem, etc.
- Reviewer of proposals for the ERC, NSF (USA), DFG (Germany), NWO (Netherlands), PRACE (Europe), FWF (Austria), ANR (France), Marsden Fund (New Zealand), NCN (Poland), and CONACYT (Mexico).
- Referee for Ph.D. thesis of Andris Gulans (Aalto University), Stephan Steinmann (EPFL), Keld Lundgaard (DTU, Denmark), Lucia Rodrigo (UAM, Madrid), Mario Zic (Trinity College Dublin); Referee for M.Sc. thesis of Stefan Chmiela (TU-Berlin).
- Top 20 Referee for 2012, designated by the *Journal of Chemical Physics*.
- Organizer of 15 international conferences and workshops.
- Proponent and chair of a semester program on “Understanding Many-Particle Systems with Machine Learning”, Institute of Pure and Applied Mathematics, University of California Los Angeles, USA.

LIST OF KEY FUNDED PROJECTS

Academic projects

Project name /Topic	Funding agency	Years	Role	Budget (k€)
VDW-CMAT Van der Waals Interactions	ERC	2011-2016	PI	1450
SMALL Organic/inorganic interfaces	Marie Curie EU	2010-2013	PI	450
CCS Machine Learning in Chemistry	DFG	2014-2017	PI	220
Dispersion Van der Waals in Molecular Crystals	DFG Priority Program	2015-2018	PI	250
HIOS-ThZ ThZ response in organic/inorganic systems	DFG-SFB	2015-2019	PI	380
IMASC Mesoporous catalysts	Department of Energy (DOE) EFRC	2014-2018	PI	250
BeStMo Quantum fluctuations in complex environments	ERC	2017-2022	PI	1840

APPENDIX

PHD SUPERVISIONS (9 IN BOLD)

Name	Type	Topic	Years	Co publis	Career
Guo-Xu Zhang	PhD	Van der Waals in solids	2010-2014	5	Ass. Prof. at HIT (Harbin Institute of Technology, China)
Javier Camarillo-Cisneros	PhD visitor	Adsorption on stepped surfaces	2011-2014	2	Researcher at Cinvestav, Chihuahua (Mexico)
Xiaofei Liu	PhD visitor	Metal-organic networks	2014-2015	1	Ass. Prof. at Nanjing University of Science and Technology, China
Victor Ruiz	PhD	Van der Waals in interfaces	2011-2016	6	Postdoc at HU Berlin
Vivekanand Gobre	PhD	Electronic structure methods	2011-2016	4	Lecturer in Pune, India
Nicola Ferri	PhD	Van der Waals and electronic properties	2011-2016	5	Postdoc at FHI Berlin
Jan Hermann	PhD	Many-body methods	2013-2017	5	PhD
Johannes Hoja	PhD	Van der Waals Entropy	2014-2018	3	PhD
Martin Stöhr	PhD	Bio-systems	2016-2020	0	PhD
Reza Karimpour	PhD	Casimir effect	2016-2020	0	PhD
Wei Liu	Post doc	Catalysis, interfaces	2010-2014	11	Professor in Nanjing University of Science and Technology, China
Wang Gao	Post doc	Defects, friction	2013-2015	4	Professor in Jilin University, China
Alberto Ambrosetti	Post Doc	Many-body methods	2012-2014	5	Lecturer at University of Padova, Italy
Katja Hansen	Post Doc	Machine learning	2012-2013	3	Researcher in 3M, Duesseldorf
Anthony Reilly	Post Doc	Molecular crystals	2012-2013	6	Professor at City University of Dublin
Igor Poltavsky	Post doc	Nuclear quantum effects	2012-	5	Senior Researcher
Mausumi Chattopadhyaya	Post Doc	Wetting	2014-2017	2	Postdoc
Fairoja Cheenicode-Kabeer	Post Doc	Catalysis	2015-2017	3	Postdoc
Gionni Marchetti	Post Doc	Machine Learning	2014-2016	1	Postdoc in Riga

Limin Zheng	Post Doc	Nuclear quantum effects	2015-	1	Visiting professor
Mainak Sadhukhan	Postdoc	Exotic van der Waals effects	2016-	1	Postdoc
Yasmine Al-Hamdani	Postdoc	Nanomaterials	2017-	1	Postdoc
Dennis Barton	Postdoc	Screened exchange	2017-	0	Postdoc
Dmitry Fedorov	Postdoc	Berry phase in molecular systems	2017-	0	Postdoc