Noé, **Frank**, Prof. Dr., May 13, 1975, male

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Position Professor (W3), tenured

University training Computer Science (2000–2002), Cork Institute of Technology, Cork, Ireland, Master of Science, Dr. Paul Rothwell
Electrical Engineering (1996–1999), University of cooperative education, Stuttgart, Germany, Dipl.-Ing. (BA), Prof. Dr. Alexander Götz.

Advanced academ. qualifications Ph.D.: Computer Science and Theoretical Biophysics (Summa Cum Laude), University of Heidelberg, Germany, 2007, Prof. Dr. Jeremy Smith

Postgraduate professional career

2015–	Adjunct Professor, Dept. of Chemistry, Rice University, Houston TX, US
2013–	Professor and Chair, FU Berlin - Joint Position between the departments of Mathematics, Physics, and Chemistry
2007–2013	Independent Junior Group Leader, DFG Centre MATHEON, FU Berlin, DE
2009–2010	Visiting professor for scientific computing, IWR/University of Heidelberg, DE
2006–2007	Postdoctoral researcher, IWR/University of Heidelberg, DE

Editorship

2019–	Editor, Machine Learning: Science and Technology (IOPscience)
2019–	Editorial Advisory Board, Journal of Chemical Theory and Computation (ACS)
2020–	Editorial Advisory Board, Journal of Chemical Physics (AIP)

Advisory boards

2021–	Scientific Advisory Board, 1qbit Inc., Canada
2020–	Executive Board, MATH+, the Berlin Mathematics Center
2020–	Scientific Advisory Board, Redesign Science Inc., USA
2014–	(Extended) Executive Board, CRC1114, FU Berlin
2012–	Faculty Member, Berlin Mathematical School (BMS)
2009–2012	Founding director, CECAM node at FU Berlin
2008–	Faculty Member, International Max Planck Research School CBSC, Berlin

Awards

2021	Elected member in the Berlin-Brandenburg Academy of Sciences
2019–2021	ISI Highly Cited Researcher (Web of Science / Clarivate)
2019	Fellow, European Laboratory for Learning and Intelligent Systems (ELLIS)
2019	Simons Fellow at the Institute of Pure and Applied Mathematics (IPAM)
2019	Early-Career Award in Theoretical Chemistry, Americal Chemical Society (ACS)
2017	ERC Consolidator Grant
2012	ERC Starting Grant
2007	Fellow, "Elite program for postdocs", Federal Foundation of Baden-Württemberg
2006	Postdoctoral fellowship, "Modelling and Simulation in the Biosciences" (BIOMS)

Peer-reviewed publications and books.

[1] J. Hermann, Z. Schätzle, and F. Noé. Deep neural network solution of the electronic schrödinger equation. *Nat. Chem.*, 12:361–390, 2020.

[2] A. Mardt, L. Pasquali, H. Wu, and F. Noé. Vampnets: Deep learning of molecular kinetics. *Nat. Commun.*, 9:5, 2018.

[3] F. Noé, S. Olsson, J. Köhler, and H. Wu. Boltzmann generators - sampling equilibrium states of many-body systems with deep learning. *Science*, 365:eaaw1147, 2019.

[4] F. Noé, C. Schütte, E. Vanden-Eijnden, L. Reich, and T. R. Weikl. Constructing the full ensemble of folding pathways from short off-equilibrium simulations. *Proc. Natl. Acad. Sci. USA*, 106:19011–19016, 2009.

[5] F. Noé, A. Tkatchenko, K. R. Müller, and C. Clementi. Machine learning for molecular simulation. *Annu. Rev. Phys. Chem.*, 71:361–390, 2020.

[6] S. Olsson, H. Wu, F. Paul, C. Clementi, and F. Noé. Combining experimental and simulation data of molecular processes via augmented markov models. *Proc. Natl. Acad. Sci. USA*, 114:8265–8270, 2017.

[7] N. Plattner, S. Doerr, G. D. Fabritiis, and F. Noé. Protein-protein association and binding mechanism resolved in atomic detail. *Nat. Chem.*, 9:1005–1011, 2017.

[8] J.-H. Prinz, H. Wu, M. Sarich, B. G. Keller, M. Senne, M. Held, J. D. Chodera, C. Schütte, and F. Noé. Markov models of molecular kinetics: Generation and validation. *J. Chem. Phys.*, 134:174105, 2011.

[9] J. Wang, S. Olsson, C. Wehmeyer, A. Peŕez, N. E. Charron, G. De Fabritiis, F. Noe, and C. Clementi. Machine learning of coarse-grained molecular dynamics force fields. *ACS Cent. Sci.*, 5:755–767, 2019.

[10] H. Wu, F. Paul, C. Wehmeyer, and F. Noé. Multiensemble markov models of molecular thermodynamics and kinetics. *Proc. Natl. Acad. Sci. USA*, 113:E3221–E3230, 2016. doi:10.1073/pnas.1525092113.