

The Harry Emmett Gunning Lecture Series was established to recognize the contributions of Professor Gunning to the Department of Chemistry from 1957 to 1974. Previous Harry Emmett Gunning Lecturers were:

M. A. Johnson	(2015)	R. N. Zare	(1998)
T. J. Martinez	(2013)	W. L. Jorgensen	(1997)
M. Fayer	(2012)	R. J. Saykally	(1995)
M. Pruski	(2011)	S. A. Rice	(1994)
G. Meijer	(2010)	H. B. Gray	(1993)
G. Richmond	(2009)	J. F. Holzwarth	(1992)
M. Gruebele	(2008)	G. R. Fleming	(1991)
M. S. Gordon	(2007)	H. F. Schaefer	(1990)
P. H. Vaccaro	(2006)	A. H. Zewail	(1989)
C. Robinson	(2005)	W. Klemperer	(1988)
M. A. Ratner	(2004)	R. R. Ernst	(1987)
J. P. Klinman	(2003)	J. N. Pitts, Jr.	(1986)
C. J. Jameson	(2002)	K. S. Pitzer	(1985)
G. Scoles	(2001)	P. M. Rentzepis	(1984)
R. M. Hochstrasser	(2000)	M. Calvin	(1983)
H. Kroto	(1999)		

The Harry Emmett Gunning Lectures replace those of the Edward Herbert Boomer Lectures that were devoted to physical-theoretical chemistry and were given by:

R. A. Marcus	(1982)
E. Clementi	(1980)
K. J. Laidler	(1978)
M. Eigen	(1976)
G. Herzberg	(1974)
A. D. Buckingham	(1972)
G. C. Pimentel	(1970)
H. S. Frank	(1967)
S. Huzinaga	(1964)
F. S. Dainton	(1962)
E. W. R. Steacie	(1958)

*You are cordially invited to attend the  
2018 Harry Emmett Gunning Lectures  
in the Department of Chemistry at the University of Alberta.*

## *The Harry Emmett Gunning Lecture Series*



**Professor Frank Neese**

*Max-Planck-Institut für Kohlenforschung  
Mülheim an der Ruhr, Germany*

**30 January – 1 February 2018**

*Physical Division, Department of Chemistry  
University of Alberta, Edmonton, Alberta*

## *Professor Frank Neese*

Frank Neese received both his Diploma (Biology – 1993) and Ph.D (Dr. rer. Nat. – 1997) working with Prof. P. Kroneck at the University of Konstanz. He performed postdoctoral work at Stanford University with Prof. E. I. Solomon from 1997 to 1999, then returned to Konstanz where he completed his Habilitation in 2001. He joined the Max Planck Institute (MPI) for Bioinorganic Chemistry in 2001 as a group leader, where he directed a research group until accepting the position of full Professor and Chair of Theoretical Chemistry at the University of Bonn in 2006. In 2008, Neese returned part time to the MPI as one of its rare “Max Planck Fellows” within the Department of Inorganic Chemistry. In 2011, he became Director of the MPI for Bioinorganic Chemistry, renamed in 2012 in MPI for Chemical Energy Conversion, where he heads the Department of Molecular Theory and Spectroscopy. Effective January 2018, he moved the Department to the neighboring MPI for Coal Research that is largely focused on all aspects of catalysis. In 2005, Neese received the Hellmann Award of the German Theoretical Chemical Society for the Development and Application of new Theoretical Methods and subsequently the Klung-Wilhelmy Weberbank Award in 2008 and the Gottfried Wilhelm Leibniz Award of the German Science Foundation in 2010. In 2013, he was inducted into the Leopoldina Nationale Akademie der Wissenschaften (German National Academy of Sciences). He was Associate Editor (2011-2014) of the journal *PhysChemChemPhys* and is a Member of the International Academy of Quantum Molecular Sciences (IAQMS, since 2012). Since 2015 Frank Neese was Associate Editor of the journal *Inorganic Chemistry* and as of 2016 he has been a Member of the Editorial Board of the review book series *Structure and Bonding*. As of 2016 Neese was appointed as an active member of the International Advisory Board for the Institute of Organic Chemistry and Biochemistry (IOCB) of the Czech Academy of Sciences in Prague and was elected as a new Member of the Review Board “Physical and

Theoretical Chemistry“ in the field of “General Theoretical Chemistry“ of the Deutsche Forschungsgemeinschaft (German Research Foundation, DFG). Frank Neese is the author of more than 440 scientific articles in journals of Chemistry, Biochemistry and Physics. His work focuses on the Theory of Magnetic Spectroscopies (electron paramagnetic resonance, magnetic circular dichroism) and their experimental and theoretical application, local pair natural orbital correlation theories, spectroscopy oriented configuration interaction, electronic and geometric structure and reactivity of transition metal complexes and metalloenzymes. He is lead author of the ORCA program.

<https://www.kofo.mpg.de/en/research/molecular-theory-and-spectroscopy>

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### LECTURE TOPICS:

**General audience: “Combining advanced spectroscopy and quantum chemistry to obtain insight into the reactivity of non-heme iron centers”**

Tuesday, 30 January 2018 at 3:00 pm, CCIS L1-140

**“Ab initio ligand field theory: a powerful tool for understanding the coordination- and magnetochemistry of d- and f-block elements”**

Wednesday, 31 January 2018 at 3:00 pm, Chemistry E1-60

**“Linear scaling local correlation methods for the accurate calculation of large systems: status and perspectives”**

Thursday, 1 February 2018 at 3:00 pm, CCIS L1-140

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