

CURRICULUM VITAE

DANIELE MACUGLIA (Chinese: 马大年)

Department of History of Science, Technology and Medicine
Academy for Advanced Interdisciplinary Studies, room 206
Peking University, Beijing, 100871, China
+86-131-4600-9849
E-Mail Address: daniele@pku.edu.cn

CURRENT POSITION

2021- Assistant Professor, Dept. of History of Science, Technology and Medicine, Peking University.

EDUCATIONAL BACKGROUND

2010-2016 University of Chicago, Ph.D. History of Science
2009-2010 University of Chicago, M.A. History of Science (MAPSS)
2003-2009 *Istituto Universitario di Studi Superiori IUSS* (Pavia)
Diploma di Licenza, Science and Technology Studies
2006-2009 University of Pavia, Department of Physics
“Summa cum Laude” (110/110 e lode) M.Sc. Physics
2003-2006 University of Pavia, Department of Physics
“Summa cum Laude” (110/110 e lode) B.Sc. Physics

EMPLOYMENT RECORD

2018-21 Research Fellow, University of Chicago (Stevanovich Institute and Neubauer Collegium)
2016-20 Lead Data Analyst, “Galileo Correspondence Project,” Stanford University

FIELD OF SPECIALIZATION

History of molecular simulations and computational statistical mechanics.

I specialize in the history of molecular simulations, which exploit computational methods to elucidate the behavior of complex atomic and molecular systems. These techniques, rooted in statistical mechanics, facilitate predictions of molecular structures, stabilities, and reaction mechanisms that are often difficult to derive experimentally. My research focuses on the theoretical physics underlying Monte Carlo and molecular dynamics methods. I actively collaborate with eminent scientists from the pivotal era of the 1970s to the early 2000s, a period that marked the emergence and consolidation of molecular simulations. My goal is not only to grasp and apply the foundational principles and insights championed by these pioneers but also to frame their historical narrative, capturing the challenges they surmounted, their aspirations, and ensuring the enduring legacy of their invaluable contributions.

PUBLICATIONS

14. “Free-Energy Calculations in Soft and Hard Matter: From Early Challenges to the Advent of Umbrella Sampling” (in preparation).
13. “Molecules, Materials and Migration: Sidney Yip’s Role in Molecular Simulations, Cold War Materials Science, and Chinese Scientific Ascendancy, 1965-1985” (currently revising, *Historical Studies in the Natural Sciences*).
12. “Melting of Silicon, 1985–1989: A New Era of Molecular Simulations,” (under review, *ISIS*).
11. “SHAKE and the Exact Constraint Satisfaction of the Dynamics of Semi-Rigid Molecules in Cartesian Coordinates, 1973-1977,” *Archive for History of Exact Sciences* 77 (2023).
10. “The Emergence of Protein Dynamics Simulations: How Computational Statistical Mechanics Met Biochemistry,” with Benoît Roux and Giovanni Ciccotti. *European Physical Journal H* 47: article number 13 (2022).
9. “The Universe: A Book Written in the Mathematical–and the Programming–Language,” *Il Nuovo Cimento* 44, No. 1 (2021).
8. “The breakthrough of a quantum chemist by classical dynamics: Martin Karplus and the birth of computer simulations of chemical reactions,” with Benoît Roux and Giovanni Ciccotti. *European Physical Journal H* 46, No. 12 (2021).
7. “Sense experiences and ‘necessary simulations:’ four centuries of scientific change from Galileo to fundamental computer simulations,” with Benoît Roux and Giovanni Ciccotti, *KNOW: A Journal on the Formation of Knowledge* 4, No. 1 (2020): 63–87.
6. “Newtonianism and information control in Rome at the wake of the eighteenth century,” *Annals of Science* 77, No. 1 (2020): 108-126.
5. “Talking about secrets: The Hanford Nuclear Facility and news reporting of silence, 1945-1989,” in Felicity Mellor and Stephen Webster, eds., *The Silences of Science. Gaps and Pauses in the Communication of Science* (London & New York: Routledge, 2017): 115-134.
4. “The work of the Roman Newtonians in the Italian Enlightenment,” in *Viewpoint, Magazine of the British Society for the History of Science* 108 (2015): 8–9.
3. “Corrado Gini and the scientific basis of fascist racism,” *Medicina nei Secoli Arte e Scienza* 26, No. 3 (2014): 821–856.
2. “Hanford and the middle ground between ‘knowing’ and ‘not knowing,’” *Bulletin of the Atomic Scientists*, “Voices of Tomorrow,” Oct. 31, 2013.
1. (in German) “Die nukleare Anlagen von Hanford (1943-1987): Eine Fallstudie über die Schnittstellen von Physik, Biologie und die US-amerikanische Gesellschaft zur Zeit des Kalten Krieges,” in Christian Forstner and Dieter Hoffmann, eds., *Physik im Kalten Krieg* (Berlin: Springer Spektrum, 2013): 77–87.

TALKS

I have presented scholarly lectures at various institutions. These include Peking University, University of Tokyo, Kyoto University, Harvard University, University of Cambridge, Imperial College London, Fermilab, and the University of Minnesota. For a comprehensive overview, please refer to my personal website: www.danielemacuglia.com.

TEACHING

History of Physics and Computational Methods; Science, Technology, and Society; Historical Methods; History of Western Science, Technology, and Medicine.

AWARDS

I received a Special Award at the “European Union Contest for Young Scientists” and the first prize at the Italian national contest “I Giovani e le Scienze” (2001). I received an honorable mention at the Italian National Physics Olympiads (2003). I was awarded the prize for best communication in the History of Physics at the 106th National Conference of the Italian Physical Society (2020).