Curriculum Vitae

Arup Sarkar

Postdoctoral Researcher
Max Planck Institute for Polymer Research
Polymer Theory Department, Ackermannweg, 10, 55128, Mainz, Germany
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Date of birth: 26th September 1991
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Research Interests

- Computational Chemistry/Electronic Structure
- Molecular Magnetism and Qubits
- Actinides/Lanthanides/Transition Metals
- Multi-reference Calculations- CASSCF/NEVPT2/CASPT2/MC-PDFT/DMRG
- Periodic DFT Calculations in Metal-Organic Frameworks and Perovskites

Research Experience

- **November 2023- present: Postdoctoral Researcher at Max Planck Institute for Polymer Research, Mainz, Germany, Supervisor: Prof. Denis Andrienko**
- **October 2021- September 2023: Postdoctoral Researcher at The University of Chicago, Department of Chemistry, 5735 S Ellis Ave, Chicago, IL 60637, US. Supervisor- Prof. Laura Gagliardi**
- **March 2021-August 2021: Institute Postdoctoral Fellow at IIT Bombay, Supervisor: Prof. Gopalan Rajaraman, Indian Institute of Technology Bombay, Mumbai, Maharashtra, India**
- August 2020- February 2021- Research Associate at IIT Bombay
- September 2018-November 2018- Visiting student at the University of Edinburgh, School of Chemistry with Prof. Euan K. Brechin
- **August 2017 to July 2020: PhD as Senior Research Fellow (CSIR) at IIT Bombay**
- **July 2015 to July 2017: PhD as Junior Research Fellow (CSIR) at IIT Bombay**
- **Thesis Title**: *Ab initio* and DFT Investigation of Electronic Structure and Spin-Hamiltonian Parameters in Transition Metal and Lanthanide-based Complexes with External Perturbations, **Supervisor: Prof. Gopalan Rajaraman**

Education

- **August 2012 - June 2014: Master of Science in Chemistry (Inorganic Specialization) Rajabazar Science College, University of Calcutta, West**

Bengal, India. Thesis Title: Synthesis, Characterization and Application of Copper Schiff-Base Complexes, **Supervisor**: **Prof. Debasis Das**

- **July 2009 - June 2012: Bachelor of Science in Chemistry (Hons.), Seth Anandram Jaipuria College, University of Calcutta, Kolkata, West Bengal, India**

Book Chapter

Ab Initio Modelling of Lanthanide-Based Molecular Magnets: Where to from Here?.

Dey, S., Sharma, T., **Sarkar, A.**, Rajaraman, G. (2023). In: Rajaraman, G. (eds) Computational Modelling of Molecular Nanomagnets. Challenges and Advances in Computational Chemistry and Physics, vol 34. Springer, Cham. https://doi.org/10.1007/978-3-031-31038-6_7.

List of Publications

1) **Probing the origin of the giant magnetic anisotropy in trigonal bipyramidal Ni(II) under high pressure**

   Gavin A. Craig**, Arup Sarkar,** Christopher H. Woodall, Moya A. Hay, Katie E. R. Marriott, Konstantin V. Kamenev, Stephen A. Moggach, Euan K. Brechin, Simon Parsons, Gopalan Rajaraman and Mark Murrie*, *Chem. Sci.* **2018,** *9*, 1551.

2) **Deciphering the origin of invariance in magnetic anisotropy in {$Fe^{II}S_4$} complexes: a theoretical perspective**

   Arup Sarkar, Gunasekaran Velmurugan, Thayalan Rajeshkumar, Gopalan Rajaraman*, *Dalton Trans.* **2018**, *47,* 9980.

3) **Trapping of a Pseudotetrahedral $Co^{II}O_4$ Core in Mixed-Valence Mixed-Geometry [Co5] Coordination Aggregates: Synthetic Marvel, Structures, and Magnetism**

   Krishna Chattopadhyay, María Jośe Heras Ojea, **Arup Sarkar**, Mark Murrie, Gopalan Rajaraman and Debashis Ray* *Inorg. Chem.* **2018**, *57*, 13176.

4) **Role of Ab Initio Calculations in the Design and Development of Organometallic Lanthanide-Based Single-Molecule Magnets**

   Abinash Swain, **Arup Sarkar**, Gopalan Rajaraman*, *Chem. Asian. J.* **2019**, *14*, 4056.

5) **In-depth investigation of large axial magnetic anisotropy in monometallic 3d complexes using frequency domain magnetic resonance and ab initio methods: a study of trigonal bipyramidal Co(II)**

   Moya A Hay, **Arup Sarkar**, Gavin A. Craig, Lakshmi Bhaskaran, Joscha Nehrkorn, Mykhailo Ozerov, Katie E. R. Marriott, Claire Wilson, Gopalan Rajaraman, Stephen Hill and Mark Murrie *Chem. Sci.* **2019**, 10, 6354.

6) **Investigation of the magnetic anisotropy in a series of trigonal bipyramidal Mn(II) complexes**

   Moya A. Hay, **Arup Sarkar**, Katie E. R. Marriott, Claire Wilson, Gopalan Rajaraman and Mark Murrie, *Dalton Trans.* **2019**, *48*, 15480.

7) **Oxidation behavior of intramolecularly coordinated unsymmetrical diorganotellurides: isolation of novel tetraorganoditelluronic acids, $[RR'Te(\mu\text{-}O)(OH)_2]_2$**

   Anand Gupta, Rajesh Deka, **Arup Sarkar**, Harkesh B. Singh and Ray J. Butcher, *Dalton Trans.* **2019**, *48*, 10979.

8) **Magnetic Anisotropy in $Co^{II}X_4$ (X=O, S, Se) Single-Ion Magnets: Role of Structural Distortions versus Heavy Atom Effect**
Arup Sarkar, Subrata Tewary, Shwetali Sinkar and Gopalan Rajaraman *Chem. Asian J.* **2019**, *14*, 4696.

9) **Isolation of Homoleptic Dicationic Tellurium and Monocationic Bismuth Analogues of Non-N-Heterocyclic Carbene Derivatives**
Rajesh Deka, **Arup Sarkar**, Ray J. Butcher, Peter C. Junk, David R. Turner, Glen B. Deacon and Harkesh B. Singh, *Organometallics* **2020**, *39*, 334.

10) **Synthesis, Characterization, and Theoretical Studies of cis-Dichloridobis(8-quinolinethiolato)tin(IV) and bis(8-Sulfanylquinolinium) Hexachloridostannate(IV)**
Rajesh Deka, **Arup Sarkar**, Harkesh B. Singh, Peter C. Junk, David R. Turner and Glen B. Deacon*, *Aust. J. Chem.* **2020**, *73*, 1128-1137.

11) **Exploring the Role of Strong Intramolecular Coordination of the 2-(2'-pyridyl)phenyl Group in Heavy Main Group Halides: Insights from Synthesis, Structural, and Bonding Analyses**
Rajesh Deka, **Arup Sarkar**, Anand Gupta, Ray J. Butcher, Peter C. Junk, David R. Turner, Glen B. Deacon and Harkesh B. Singh*, *Eur. J. Inorg. Chem.* **2020**, *22*, 2143.

12) **Isolation of the novel example of a monomeric organotellurinic acid**
Rajesh Deka, **Arup Sarkar**, Ray J. Butcher, Peter C. Junk, David R. Turner, Glen B. Deacon and Harkesh B. Singh*, *Dalton Trans.* **2020**, *49*, 1173.

13) **Halogenation of Diorganotelluride $[2,6\text{-}(Me_2NCH_2)_2C_6H_3]Te$*n*Bu: Synthesis, Molecular and Electronic Structural Investigation of Monoorgano Dihalotelluronium(IV) Cation**
Rajesh Deka, Anand Gupta, **Arup Sarkar**, Ray J. Butcher and Harkesh B. Singh*, *Eur. J. Inorg. Chem.* **2020**, *44*, 4170-4179.

14) **Influence of ligand field on magnetic anisotropy in a family of pentacoordinate Co^{II} complexes**
Joydev Acharya, **Arup Sarkar**, Pawan Kumar, Vierandra Kumar, Jessica Flores Gonzalez, Olivier Cador, Fabrice Pointillart, Gopalan Rajaraman and Vadapalli Chandrasekhar*, *Dalton Trans.* **2020**, *49*, 4785.

15) **A large axial magnetic anisotropy in trigonal bipyramidal Fe(II)**
Moya A. Hay, **Arup Sarkar**, Gavin A. Craig, Katie E. R, Marriott, Claire Wilson, Gopalan Rajaraman and Mark Murrie*, *Chem Commun.* **2020**, *56*, 6826.

16) **Role of Coordination Number and Geometry in Controlling the Magnetic Anisotropy in Fe(II), Co(II) and Ni(II) Single-Ion Magnets**
Arup Sarkar, Sourav Dey and Gopalan Rajaraman*, *Chem. Eur. J.* **2020**, *26, 14036-14058.*

17) **Modulating magnetic anisotropy in Ln(III) single-ion magnets using an external electric field**
Arup Sarkar and Gopalan Rajaraman*, *Chem. Sci.* **2020**, *11, 10324.*

18) **Chiral Tetranuclear Copper(II) Complexes: Syntheses, Optical and Magnetic Properties**
Naushad Ahmed, Shalini Tripathi, **Arup Sarkar**, Kamal Uddin Ansari, Chinmoy Das, Neetu Prajesh, Satoshi Horike, Ramamoorthy Boomishankar and Maheswaran Shanmugam *New J. Chem.,* **2020**, *44, 16845.*

19) **Modulation of Magnetic Anisotropy and Exchange Interaction in Phenoxide Bridged**

Dinuclear Co(II) complexes

Ajit Kumar Kharwar, Arpan Mondal, **Arup Sarkar**, Gopalan Rajaraman and Sanjit Konar*, *Inorg. Chem.* **2021***, 60,* 11948−11956.

20) **$[(V^{IV}O)_2M^{II}_5]$ (M= Ni, Co) Anderson wheels**

Hector W. L. Fraser, Emily Payne, **Arup Sarkar**, Lucinda R. B. Wilson, Dmitri Mitcov, Gary S. Nichol, Dimitrios Kampouris, Gopalan Rajaraman, Stergios Piligkos and Euan K. Brechin*, *Dalton Trans.* **2021***, 50,* 12495-12501.

21) **Exploiting Host-Guest Chemistry to Manipulate Magnetic Interactions in Metallosupramolecular M_4L_6 Tetrahedral Cages**

Aaron J. Scott, Julia Vallejo, **Arup Sarkar**, Lucy E. Smythe, E. Regincós Martí, Gary S. Nichol, Wim T. Klooster, Simon J. Coles, Mark Murrie, Gopalan Rajaraman, Stergios Piligkos, Paul J. Lusby and Euan K. Brechin*, *Chem Sci.* **2021***, 12, 5134.*

22) **Record High Magnetic Anisotropy in Three Coordinated Mn^{III} and Cr^{II} Complexes: A Theoretical Perspective**

Arup Sarkar, Reshma Jose, Harshit Ghosh and Gopalan Rajaraman* *Inorg. Chem.* **2021**, *60*, 9680−9687.

23) **Electric field-induced solid-gas interfacial chemical reaction in carbon nanotubes ensembles: Route towards ultra-sensitive gas detectors**

Itisha Dwibedi, **Arup Sarkar**, Gopalan Rajaraman and Chandramouli Subramaniam*, *ACS Appl. Mater. Interfaces* **2022**, 14, 13271−13279.

24) **What Controls the Magnetic Anisotropy in Heptacoordinate High-Spin Cobalt(II) Complexes? - A Theoretical Perspective**

Peter Comba*, Gopalan Rajaraman, **Arup Sarkar,** Gunasekaran Velmurugan, *Dalton Trans.* **2022**, 51, 5175-5183**.**

25) **Implementing the Ambiphilicity of an Organotellurenyl Cation for the Synthesis of a Platinum (II)-Based Carboxylate-Bridged Heterobimetallic Complex: Structure and Bonding Analysis**

Rajesh Deka*, **Arup Sarkar,** Ray J. Butcher and Harkesh B. Singh, *Eur. J. Inorg. Chem.* **2022***, e202200403.*

26) **Multiconfiguration Pair-Density Functional Theory for Chromium (IV) Molecular Qubits**

Arturo Sauza-de la Vega, Riddhish Pandharkar, Gautam D Stroscio, **Arup Sarkar**, Donald G Truhlar, Laura Gagliardi*, *JACS Au* **2022***, 2,* 2029−2037**.**

27) **Linker Redox Mediated Control of Morphology and Properties in Semiconducting Iron-Semiquinoid Coordination Polymers**

Lei Wang, Robert J. Papoular, Noah E. Horwitz, Jiaze Xie, **Arup Sarkar**, Dario Campisi, Norman Zhao, Baorui Cheng, Garrett L. Grocke, Tengzhou Ma, Alexander S. Filatov, Laura Gagliardi, and John S. Anderson*, *Angew. Chem. Int. Ed.* **2022***, 61,* e202207834**.**

28) **The Role of Metal Selection in the Radiation Stability of Isostructural M-UiO-66 Metal–Organic Frameworks**

Ashley M. Hastings, Melissa Fairley, Megan C. Wasson, Dario Campisi, **Arup Sarkar**, Zoë C. Emory, Kieran Brunson, Dylan B. Fast, Timur Islamoglu, May Nyman, Peter C. Burns, Laura Gagliardi, Omar K. Farha, Amy E. Hixon, and Jay A. LaVerne*, *Chem. Mater.* **2022***, 34,* 8403−8417.

29) **Theoretical Investigation of Single-Molecule Magnet Behavior in Mononuclear Dysprosium and Californium Complexes**

Debmalya Ray, Meagan S. Oakley, **Arup Sarkar,** Xiaojing Bai, and Laura Gagliardi*, *Inorg. Chem.*, **2023,** 62, 4, 1649–1658**.**

30) **Broad Electronic Modulation of 2D Metal-Organic Frameworks Over Four Distinct Redox States**

Lei Wang, **Arup Sarkar**, Garrett L. Grocke, Daniel William Laorenza, Baorui Cheng, Andrew Ritchhart, Alexander S. Filatov, Shrayesh N. Patel, Laura Gagliardi, and John S. Anderson* **2023** *J. Am. Chem. Soc.* **2023**, *145*, 8486−8497**.**

31) **Understanding Antiferromagnetic and Ligand Field Effects on Spin Crossover in a Triple-decker Dimeric Cr(II) Complex**

Arup Sarkar, Matthew R. Hermes, Christopher J. Cramer, John S. Anderson and Laura Gagliardi*, *J. Am. Chem. Soc.* **2023,** *145*, 22394–22402.

32) **Elucidating actinide-pertechnetate and actinide-perrhenate bonding via a family of Th-TcO4 and Th-ReO4 frameworks and solutions**

Mohammad Shohel, Jenna Bustos, Gautam D. Stroscio, **Arup Sarkar**, May Nyman*, *Inorg. Chem.* **2023**, *62*, 10450−10460.

33) **Multiconfiguration pair-density functional theory for the vertical excitation energies in actinide molecules**

Arup Sarkar, Laura Gagliardi* *J. Phys. Chem. A*, **2023**, 127, 9389.

34) **Theoretical study of the formation of metal–oxo species of the first transition series with the ligand 14-TMC: driving factors of the "Oxo Wall"**

Monika, Manjeet Kumar, Somi, **Arup Sarkar**, Manoj Kumar Gupta and Azaj Ansari* *Dalton Trans.*, **2023**, 52, 14160-14169.

Projects

At IIT Bombay, with Prof. Gopalan Rajaraman

Department of Chemistry, Indian Institute of Technology-Bombay, India **(July 2015-Dec 2020)**

The primary objective of my research deals with the investigation of the origin of magnetic anisotropy and magnetic exchange in transition metal and lanthanide metal-based systems with various multireference quantum chemical methods such as- DFT, CASSCF, CASPT2, State Interaction Spin-Orbit Coupling. Some of the important projects are:

- Deciphering the origin of magnetic anisotropy in mononuclear 3d transition metal systems and identifying the major structural parameter which can fine-tune the zero-field splitting parameters. Developing a magneto-structural correlation with the important structural parameters obtained from frequency calculations.
- Exploring the origin of magnetic anisotropy in di-, tri- and polynuclear transition metal systems involving strong metal-metal bonded systems and the importance of spin-flipped electronic

excitations in these complexes.

- Modulating magnetic anisotropy in Ln(III) mononuclear coordination complexes using an external electric field.

Visiting research scholar (student exchange program under UGC-UKEIRI program), University of Edinburgh, School of Chemistry, Scotland, UK (September 2018-November 2018)

Supervisor: **Prof. Euan K. Brechin**

- Molecular Magnetic Materials for Qubit Applications.

At The University of Chicago, the Department of Chemistry

Supervisor: **Prof. Laura Gagliardi**

- Investigating the electronic structure and magnetic properties is solids and metal-organic frameworks using periodic DFT (PBE+U, HSE06) methods (Catalyst Design for Decarbonization Center).
- Quantum chemical treatment of strongly correlated magnetic systems based on Heavy elements (actinides, lanthanides) using MC-PDFT, HMC-PDFT and CMS-PDFT methods.
- Multi-configurational Pair Density Functional Theory (MC-PDFT) for Magnetic Systems.

At the Max Planck Institute for Polymer Research:

Supervisor: Denis Andrienko

- Insight into interfacial charge recombination processes in metal halide perovskite solar cells.

Software Expertise

Gaussian, ORCA, OpenMolcas, PySCF, VASP, CP2K, SIESTA, **Quantum Espresso**, **Atomistic Simulation Environment**, **GROMACs**, AIM2000, Multiwfn, PHI, Chemcraft, Gauss View, MOLDEN, Avogadro, Chimera, ChemDraw, Maestro (Schrodinger), Mercury.

Programming experience

LINUX, Python, Shell scripting.

Scholastic Achievements

- Qualified **Joint CSIR-UGC NET** exam in June 2014 (Rank 45).
- Qualified **GATE** exam in 2014 with an India rank 143.
- Awarded **Junior** and **Senior Research Fellowship** from the Council of Scientific and Industrial Research (CSIR) India.
- Grant Proposal accepted for **Marie Skłodowska-Curie Actions (MSCA) Fellowship** 2023-24 from Horizon Europe Framework Programme with **Prof. Alessandro Lunghi** at Trinity College Dublin, Ireland.
- Government of Ireland (GOI) Irish Postdoctoral Fellowship for 2024 -declined.
- **Alexander von Humboldt fellowship** – declined.

Conferences

- Delivered lecture in '***6th Calcutta University Post-Graduate Centenary Seminar Contest 2012***' organized by 100 years of C.U.P.G. Teaching in Chemistry, Celebration Committee, Department of Chemistry, Scottish Church College, University of Calcutta April, 2013.
- Poster presented in *"**Modern Trends in Inorganic Chemistry 2015 (MTIC-XVI)**"*, organized by Department of Chemistry, Jadavpur University, Kolkata, India, 3rd-5th December 2015.

- Poster presented in *"**Workshop on Electronic Structure of Coordination Complexes**"*, Department of Chemistry, IIT Bombay, Mumbai, India, 16th-18th May 2016**.**
- Poster presented in *"**Modern Trends in Molecular Magnetism (MTMM)**"*, Department of Chemistry, IIT Bombay, Mumbai, India, 19th-21st May 2016**.**
- Poster presented in **"*Theoretical Chemistry Symposium (TCS) India 2016*"**, organized by the Department of Chemistry, University of Hyderabad, India, December 2016.
- Poster presented in **"*Recent Advances on Many Electron Theory (RAMET) 2017*"** GOA, IACS and IIT Bombay, India, February 2017**.**
- Poster presented in **"*World Association of Theoretical and Computational Chemistry (WATOC) 2017*"** Munich, Germany, August 2017.
- Poster presented in **"*Asia Pacific Conference on Theoretical and Computational Chemistry (APCTCC) 2017*"** organized by Dept. of Chemistry, IIT Bombay, India, December 2017.
- Poster presented in **"*New Frontiers in Chemical Sciences (NFCS)*"** organized by Dept. of Chemistry, IIT Bombay, India, December 2018.
- Poster presented at ***In House Symposium***, held at IIT Bombay, Mumbai, India, February, 2019.
- Participated and poster presented in both workshop and conference **"*Advanced Simulation Methods (ASM)*"** organized by IIT Delhi, New Delhi, India, in March 2019**.**
- Poster presented in "***Modern Trends in Molecular Magnetism (MTMM) 2019***" organized by Dept. of Chemistry IISER Bhopal, Madhya Pradesh, India in November 2019.
- Oral presentation at ***American Chemical Society (ACS Fall 2022)*** in the Physical Chemistry Division, August 21-25, 2022, Chicago, IL, USA.
- Oral presentation and Presider at ***American Chemical Society (ACS Fall 2023)*** in the Lanthanides and Actinides Inorganic division, August 13-17, 2023, San Francisco, CA, USA.
- Participated and poster presented at "***Quantum Systems in Chemistry, Physics and Biology QSCP-XXVI***" organized by Ashoka University at Jaipur, Rajasthan in 2023 October.
- Attended the **SPP 2196 workshop** (Perovskite semiconductors: From fundamental properties to devices) in Feb-March 2024 at Stuttgart, Germany.

Teaching Experience

- **CH 117:** Undergraduate 1st-year Laboratory Class in Chemistry (1 Semester, 1 class/week, 80 UG Students) at IIT-Bombay in spring 2018.
- **CH 105:** Undergraduate 1st year Class in Inorganic Chemistry (1 Semester, 2 classes/week, 100 UG Students) at IIT-Bombay in autumn 2017 and autumn 2018.
- **CH 224:** Undergraduate second-year Coordination Chemistry Course (1 semester, 2 classes/week) at IIT Bombay in Spring 2017-2018.

Mentorship

- **Anindya Bakshi** (February 2020-July 2020) from Dept. of Chemical Engineering, Manipal Institute of Technology, Manipal, Karnataka, India.
- **Daniel Cutler** (October 2019-December 2019): UGC-UKIERI Exchange student from the School of Chemistry, University of Edinburgh, Scotland, UK.
- **Vishal Kumar Porwal** (May 2018- July 2018): Summer intern from IISER Mohali.
- **Sahil Dhingra** (September 2017- April 2018): BS-MS Project student at IIT Bombay.
- **Harshit Ghosh** (May 2017-July 2017): Summer intern from IIT Kanpur.

- **Natalia Lussari Vrech,** Universidade de Sao Paulo Campus da Capital: Sao Paulo, SP, BR, (January 2022- June 2022): Project student at Gagliardi group.
- **Arturo Sauza,** Graduate Student at The University of Chicago, Chicago, Illinois, (October 2022-September 2023).
- **Shwetali Sinkar,** BS-MS project student at IIT Bombay (September 2016-April 2017).

References

(1) Prof. Gopalan Rajaraman

Department of Chemistry, Indian Institute of Technology-Bombay, Powai, Mumbai-400076, India. **Email**: rajaraman@chem.iitb.ac.in, URL: http://www.chem.iitb.ac.in/~rajaraman/

(2) Prof. Laura Gagliardi

Richard and Kathy Leventhal Professor
Department of Chemistry, Pritzker School of Molecular Engineering, James Franck Institute,
Director of the Chicago Center for Theoretical Chemistry
Department of Chemistry, The University of Chicago
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Group Web Site: https://gagliardigroup.uchicago.edu

(3) Prof. Euan K. Brechin

Professor of Coordination Chemistry, EaStCHEM School of Chemistry, The University of Edinburgh, King's Buildings, David Brewster Road, Edinburgh EH9 3FJ.
Email: ebrechin@ed.ac.uk

(4) Prof. Maheswaran Shanmugam

Department of Chemistry, Indian Institute of Technology-Bombay, Powai, Mumbai-400076, India. **Email**: eswar@chem.iitb.ac.in
URL: https://kamal1607.wixsite.com/mysite

(5) Prof. Achintya Kumar Dutta

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URL: https://achintyachemist.wixsite.com/achintya/publications

(6) Prof. John S. Anderson

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Email: jsanderson@uchicago.edu
URL: https://andersonlab.uchicago.edu/

(7) Prof. Denis Andrienko

Organic Electronics Lab (Theory Group), Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany
Email: denis.andrienko@mpip-mainz.mpg.de

URL: https://www2.mpip-mainz.mpg.de/~andrienk/contact/

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