Dr. Diego Sorbelli, PhD
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Education and research experience

University of Perugia, Dep. of Chemistry, Biology, Biotechnology — Perugia, IT
Junior Assistant Professor (RTDA) in General and Inorganic Chemistry — 05/2025-present

University of Chicago, Pritzker School of Molecular Engineering — Chicago, US
Research Associate, Advisor: Prof. Giulia Galli — 05/2025-present

University of Chicago, Pritzker School of Molecular Engineering — Chicago, US
Postdoctoral Scholar, Advisor: Prof. Giulia Galli — 2023-2025

University of Perugia, Dep. of Chemistry, Biology, Biotechnology — Perugia, IT
Ph.D. in Chemical Sciences – Theoretical Chemistry and Computational Modelling (cum laude). Advisors: Prof. Paola Belanzoni, Dr. Leonardo Belpassi. — 2019-2023

Erasmus+ Research Traineeship — Toulouse, FR
Université Toulouse III – Paul Sabatier – CNRS. Advisor: Prof. Trond Saue. — 2019

University of Perugia, Dep. of Chemistry, Biology, Biotechnology — Perugia, IT
M.S. in Chemical Sciences – Joint European Master in Theoretical Chemistry and Computational Modeling (cum laude) — 2017-2019

University of Perugia, Dep. of Chemistry, Biology, Biotechnology — Perugia, IT
B.S. in Chemistry (cum laude) — 2014-2017

Teaching and mentoring experience

- Mentor of a visiting PhD student from the University of Perugia at the University of Chicago (09/2024-03/2025).
- Teaching fellow for the *General and Inorganic Chemistry*, *Fundamentals of Quantum Chemistry* and *Bioinorganic Chemistry* for the B.S. and M.S. courses in Chemistry, University of Perugia (2020-2025).
- Teaching assistant in *General and Inorganic Chemistry* – degrees in Biology and Pharmaceutical Chemistry, University of Perugia (2017-2021).
- Co-advisor of one bachelor and two master students for their final undergraduate theses, University of Perugia (2022-2023).

Publications

Number of peer-reviewed publications = **25**
Manuscripts in preparation/submitted (*)= **2**
First author publications = **19**
Main corresponding author (*) = **2**
Co-corresponding author (**) = **10**

- L. Baldinelli, **D. Sorbelli**,** M. Toriyama, G. Bistoni, F. De Angelis, G. Galli, *Design rules to engineer the spin structure of Cr(IV) molecular qubits via matrix modularity.* Submitted. ChemRxiv DOI: 10.26434/chemrxiv-2025-79sw7 *

- **D. Sorbelli**, G. Galli, *Disentangling morphological and electronic effects in polymerized acceptors for all-polymer solar cells.* Submitted*

- **D. Sorbelli**, Y. Wu, Z. Bao, G. Galli, *Mesomeric control of the optoelectronic properties of polymerized small molecule acceptors. J. Mater. Chem. A*, **2024**, *12,* 25837-25849.

- Y. Wu, Y. Yuan, **D. Sorbelli**, C. Cheng, L. Michalek, H.-W. Cheng, V. Jindal, S. Zhang, G. LeCroy, E. D. Gomez, S. T. Milner, A. Salleo, G. Galli, J. B. Asbury, M. F. Toney, Z. Bao, *Tuning polymer-backbone coplanarity and conformational order to achieve high-performance printed all-polymer solar cells. Nat. Commun.* **2024**, *15*, 2170.

- **D. Sorbelli**,** L. Belpassi, P. Belanzoni, *Coinage metal effect on the reduction of carbon dioxide with monomeric metal-hydride complexes. Eur. J. Inorg. Chem.* **2024**, e202400280.

- E. Rossi, **D. Sorbelli,*** P. Belanzoni, L. Belpassi, G. Ciancaleoni, *Monomeric gold hydrides for carbon dioxide reduction: ligand effect on the reactivity. Chem. Eur. J.* **2024**, e202303512. (*selected by the Editor as "Hot Paper"*)

- **D. Sorbelli,**** L. Belpassi, P. Belanzoni, *Cooperative small molecule activation by apolar and weakly polar bonds through the lens of a suitable computational protocol. Chem. Commun.* **2024**, 60, 1222-1238. (*selected for the "Chemical Communications HOT Articles 2024" themed collection and merited the cover picture of the journal*).

- X. Gui, **D. Sorbelli**, F.P. Caló, M. Leutzsch, M. Patzer, A. Fürstner, G. Bistoni, A. Auer, *Elucidating the Electronic Nature of Rh-based Paddlewheel Catalysts from ^{103}Rh NMR Chemical Shifts: Insights from Quantum Mechanical Calculations. Chem. Eur. J.* **2024**, 30, e202301846.

- **D. Sorbelli**, P. Belanzoni, L. Storchi, O. Bizzarri, B. Bizzarri, E. Mosconi, L. Belpassi, *Chemical bond analysis for the entire periodic table: energy decomposition and natural orbitals for chemical valence in the four-component relativistic framework. Molecular Physics*, **2023**, e2245061.

- **D. Sorbelli,**** L. Belpassi, P. Belanzoni, *Widening the Landscape of Small Molecule Activation with Gold-Aluminyl Complexes: A Systematic Study of E−H (E=O, N) Bonds, SO_2 and N_2O Activation. Chem. Eur. J.* **2023**, *29*, e202203584.

- **D. Sorbelli,**** L. Belpassi, P. Belanzoni, *Radical-like reactivity for dihydrogen activation by coinage metal-aluminyl complexes: computational evidence inspired by experimental main group chemistry. Chem. Sci.* **2023**, *14*, 889-896.

- I. F. Leach, **D. Sorbelli**, L. Belpassi, P. Belanzoni, R.W.A. Havenith, J.E.M.N. Klein, *How reduced are nucleophilic gold complexes? Dalton. Trans.* **2023**, *52*, 11-15.

- **D. Sorbelli,**** L. Belpassi, P. Belanzoni, *Mechanistic Study of Alkyne Insertion into Cu-Al and Au-Al bonds: a paradigm shift for coinage metal chemistry. Inorg. Chem.* **2022**, *61*, 51, 21095-21106.

- M. De Santis, **D. Sorbelli**, V. Vallet, A. S. P. Gomes, L. Storchi, L. Belpassi, *Frozen-Density Embedding for Including Environmental Effects in the Dirac-Kohn–Sham Theory: An Implementation Based on Density Fitting and Prototyping Techniques. J. Chem. Theory Comput.* **2022**, *18*, 10, 5992-6009.

- **D. Sorbelli,**** E. Rossi, R.W.A. Havenith, J.E.M.N. Klein, L. Belpassi, P. Belanzoni, *Gold-aluminyl and gold-diarylboryl complexes: bonding and reactivity with carbon dioxide. Inorg. Chem.* **2022**, *61*, 7327-7337.

- **D. Sorbelli,**** L. Belpassi, P. Belanzoni, *Unraveling differences in aluminyl and carbene coordination chemistry: bonding in gold complexes and reactivity with carbon dioxide. Chem. Sci.* **2022**, *13*, 4623-4634.

- **D. Sorbelli**, P. Belanzoni, L. Belpassi, J.-W. Lee, G. Ciancaleoni, *ETS-NOCV-based computational strategies for the characterization of concerted transition states involving CO_2, J. Comput. Chem.* **2022**, *43*, 717-727.

- **D. Sorbelli,**** L. Belpassi, P. Belanzoni, *What singles out aluminyl anions? A comparative computational study of the carbon dioxide insertion reaction in gold-aluminyl, -gallyl, -indyl complexes. Inorg. Chem.* **2022**, *61*, 1704–1716.

- **D. Sorbelli,**** L. Belpassi, P. Belanzoni, *Reactivity of a gold-aluminyl complex with carbon dioxide: a nucleophilic gold? J. Am. Chem. Soc.* **2021**, *143*, 14433-14437.

- **D. Sorbelli,*** P. Belanzoni, L. Belpassi, *Tuning the gold(I)-carbon bond in gold-alkynyl complexes through structural modifications of the NHC ancillary ligand: effect on spectroscopic observables and reactivity*. *Eur. J. Inorg Chem.* **2021**, *2021*, 2401-2416.

- **D. Sorbelli**, J. Segato, A. Del Zotto, L. Belpassi, D. Zuccaccia, P. Belanzoni, *The mechanism of the gold(I)-catalyzed Meyer-Schuster rearrangement of 1-phenyl-2-propyn-1-ol via 4-endo-dig cyclization*. *Dalton Trans*. **2021**, *50*, 5154-5160.

- **D. Sorbelli**, M. De Santis, P. Belanzoni, L. Belpassi, *Spectroscopic/bond property relationship in Group 11 dihydrides via relativistic four-component methods*. *J. Phys. Chem. A* **2020**, *124*, 10565-10579.

- **D. Sorbelli,**** P. Belanzoni, T. Saue, L. Belpassi, *Ground and excited electronic states of AuH_2 via detachment energies on AuH_2^- using state-of-the-art relativistic calculations*. *Phys. Chem. Chem. Phys.* **2020**, *22*, 26742-26752. (*selected by the editor as Hot Article*).

- E. Rossi, M. De Santis, **D. Sorbelli**, L. Storchi, L. Belpassi, P. Belanzoni, *Spin-orbit coupling is the key to unraveling intriguing features of the halogen bond involving astatine*. *Phys. Chem. Chem. Phys.* **2020***, 22*, 1897-1910. (*selected by the editor as Hot Article*).

- **D. Sorbelli**, L. Nunes dos Santos Comprido, G. Knizia, A. S. K. Hashmi, L. Belpassi, P. Belanzoni, J. E. M. N. Klein, *Cationic gold(I) diarylallenylidene complexes: bonding features and ligand effects. ChemPhysChem* **2019**, *20*, 1671-1679 (*merited the cover picture of the journal*).

- L. Gregori, **D. Sorbelli**, L. Belpassi, F. Tarantelli, P. Belanzoni, *Alkyne activation with gold(III) complexes: a quantitative assessment of the ligand effect by charge-displacement analysis. Inorg. Chem.* **2019**, *58*, 3115-3129.

- **D. Sorbelli**, L. Belpassi, F. Tarantelli, P. Belanzoni, *Ligand effect on bonding in gold(III) carbonyl complexes*, *Inorg. Chem.* **2018**, *57*, 6161-6175.

Awards and fellowships

- Junior *"EnerCHEM"* award – *for early career researchers (under 35 years old) with outstanding contributions in the field of chemistry for renewable energy* – awarded by the Chemistry for Renewable Energy division of the Italian Society of Chemistry (2024).
- Best PhD Thesis, awarded by the Umbria division of the Italian Society of Chemistry (2023).

- Best poster at the 13th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics (REHE 20-22).

- Fellowship to attend the 27th Conference of the Italian Chemical Society, awarded by the Theoretical and Computational Chemistry division of the Italian Chemical Society (2021).

- Fellowship for the attendance to the scientific contest "Catalisi in Gioco", awarded by the Catalysis group of the Italian Chemical Society (2021).

- PhD fellowship, awarded by the Italian Ministry of University and Research under the project *"Dipartimenti di Eccellenza 2018-2022 – AMIS project"* (2019).

Invited talks

Number of invited talks = **6**

- XXVIII National Congress of the Italian Society of Chemistry – Milan, IT, August 28th 2024.

- Gordon Research Seminar – Computational Materials Science and Engineering – Newry, ME, USA, July 20th-21st 2024 *keynote speaker)*.

- Italian Chemical Society (Umbria division) – Christmas Lectures – Perugia, Italy, December 22nd 2023.

- 2023 Organic & Perovskite Solar Cell Review – organized by Office of Naval Research, University of North Carolina, Chapel Hill, NC, USA, May 16-18th 2023.

- 1st Symposium for Young Chemists: Innovation and Sustainability (SYNC), Rome, Italy, 20th - 23rd June 2022 (*keynote speaker)*.

- 13th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics (REHE) – Virtual talks event, August 27th 2021.

Contributed talks and posters

Number of oral contributions = **9**
Number of poster contributions = **3**

- APS Global Physics Summit 2025, Anaheim, USA, 16th – 21st March 2025 (oral).

- Gordon Research Conference – Computational Materials Science and Engineering – Newry, ME, USA, July 21th-26st 2024 (poster).

- APS March Meeting, Minneapolis, USA, 3rd – 8th March 2024 (oral).

- 13th International Conference on Relativistic Effects in Heavy-Elements Chemistry and Physics (REHE 20-22), Assisi, Italy, 26-30th September 2022 (poster).

- 44th International Conference on Coordination Chemistry (ICCC), Rimini, Italy, 28th August – 2nd September 2022 (oral).

- 29th International Conference on Organometallic Chemistry (ICOMC), Prague, Czech Republic, 17th-22nd July 2022 (oral).

- Workshop of the Theoretical and Computational Chemistry division of the Italian Chemical Society, Florence, Italy, 8th April 2022 (oral).

- JAWSchem Webinar series, online webinar, 1st March 2022 (oral).

- International School on Inorganic Materials, Bardonecchia, Italy,15-18th December 2021 (oral).

- 27th Conference of the Italian Chemical Society, online, 14th-23rd September 2021 (oral).

- Virtual Conference on Organometallic Chemistry (EuCOMC XXIV), online, 1st-3rd September 2021 (poster).

- Virtual Symposuym on Chemical Theory and Computation (VS-CTC), online, 21st December 2021 (oral).

Service

- Reviewer for: *Chemistry – A European Journal, Journal of Physics: Materials, Electronic Structure, Journal of Physics D: Applied Physics, Journal of Organometallic Chemistry, Physica Scripta, Computational and Theoretical Chemistry.*

- Review Editor for *Frontiers in Chemistry* (specialty section: Theoretical and Computational Chemistry).

- Member of the local organizing committee of the *12th EuChemS Computational and Theoretical Chemistry (EuCO) conference (2019, Perugia, Italy)* and of the *13th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics (REHE, 2022, Assisi, Italy).*

- Member of the Executive Council of Pritzker School of Molecular Engineering Postdoctoral Association (PME-PDA, 2024-2025).
- Member of the 2024 University of Chicago Postdoc Advisory Board (2024).