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## Curriculum Vitae Professor Dr Àngel Rubio



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**Name:** Àngel Rubio  
**Born:** 27 September 1965

**Research Priorities:** Ultrafast phenomena in molecular and condensed systems, time-dependent functional theory for quantum electrodynamics, characterizing new non-equilibrium states of matter.

Àngel Rubio is a Spanish physicist. He develops theoretical instruments that both aid in the study of electronical reactions of materials and molecules as well as in the prediction of non-equilibrium phases of matter. He is known for his highly impactful works and leadership in computational solid-state physics, predicting novel materials properties at the nanometer scale, and, more recently, new non-equilibrium phases of matter, opening the fields of cavity materials engineering and QED-polaritonic chemistry. He is considered a pioneer of computer-aided material science and is one of the founders of modern theoretical spectroscopy.

### Academic and Professional Career

- since 2019 Co-Director, Max-Planck-New York City Center for Non-equilibrium Quantum Phenomena, New York City, USA
- since 2017 Distinguished Research Scientist, Center for Computational Quantum Physics (CCQ), Flatiron Institute, Simons Foundation, New York City, USA
- since 2017 Distinguished Honorary Professor, Condensed Matter Physics, Universidad del País Vasco UPV/EHU, San Sebastián, Spain
- since 2016 Professor, Universität Hamburg (UHH), Hamburg, Germany
- since 2014 Director and Scientific Member, Max-Planck-Institute for the Structure and Dynamics of Matter (MPSD), Hamburg, Germany (Managing Director from 2016-2019 and since 2022)
- 2014 Miller Guest Professor, University of California, Berkeley (UC Berkeley), Berkeley, USA

- 2009 - 2011 Distinguished Visiting Scientist, Fritz Haber Institute, Max-Planck Society (MPG), Berlin, Germany
- 2007 Professor, Université de Montpellier 2, Montpellier, France
- 2006 - 2006 Humboldt-Professor, Freie Universität (FU) Berlin, Berlin, Germany
- 2001 - 2014 Professor for Condensed Matter Physics and Director, Group “Nano-Bio Spectroscopy”, Universidad del País Vasco UPV/EHU, San Sebastián, Spain
- 2000 - 2001 Professor, Laboratoire des Solides Irradiés, École Polytechnique, Palaiseau, France
- 1994 - 2001 Associate Professor, Section “Física Teórica, Atomica y Nuclear”, Universidad de Valladolid, Valladolid, Spain
- 1992 - 1993 Fulbright Fellow, Department of Physics, UC Berkeley, Berkeley, USA
- 1988 - 1992 Research Fellow, Ministerio de Educación y Ciencia, Universidad Valladolid, Valladolid, Spain
- 1991 PhD in Physics, Universidad de Valladolid, Valladolid, Spain
- 1988 BSc in Physics, Universidad de Valladolid, Valladolid, Spain

#### **Functions in Scientific Societies and Committees**

- 2019 - 2023 Member, Scientific Advisory Board, Focus Area “Information”, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany
- since 2017 Co-Editor, Proceedings of the National Academy of Sciences (PNAS)
- 2017 - 2023 Co-Editor, NanoLetters ACS
- since 2015 Member, Faculty, Wolfgang Pauli Centre, Hamburg, Germany
- 2012 - 2014 Vice-President for Scientific Development, European Theoretical Spectroscopy Facility (ETSF)
- 2008 - 2014 Co-Founder and Chair, ETSF

#### **Project Coordination and Membership in Collaborative Research Projects**

- 2019 - 2025 Participating Researcher, Cluster of Excellence (EXC) 2056 “CUI: Advanced Imaging of Matter (AIM)”, German Research Council (DFG), Germany
- 2019 - 2023 Chair, Subproject “Ultrafast stabilization mediated by electronic correlations”, Collaborative Research Center (SFB) 925, DFG, Germany
- 2018 - 2021 Participating Researcher, Transnational Research Project “ERA-NET: Cofund in Quantum Technologies”, QuanTERA, Federal Ministry of Education and Research, Germany

- 2017 - 2019 Participating Researcher, Graduate School “Quantum Mechanical Materials Modelling – QM3”, DFG, Germany
- 2016 - 2021 Coordinator and Principal Investigator, Advanced Grant „QSpec-NewMat”, European Research Council (ERC)
- 2015 - 2018 Participating Researcher, Center of Excellence “The Novel Materials Discovery (NoMaD)”, Horizon 2020 Research and Innovation Programme, European Union (EU)
- 2011 - 2016 Coordinator and Principal Investigator, Advanced Grant „DYNamo”, ERC

### **Honours and Awarded Memberships**

- 2023 Premio Nacional de Investigación Blas Cabrera, Spain
- since 2023 Member, German National Academy of Sciences Leopoldina, Germany
- since 2022 Member, Berlin-Brandenburg Academy of Science (BBAW), Germany
- 2022 Alumni UvA de Honor, Universidad de Valladolid, Spain
- 2022 Highly Cited Researcher, Web of Science, Clarivate Analytics, London, UK
- 2021 Member, European Physical Society (EPS)
- 2020 Member, European Academy of Sciences
- 2018 Max-Born Award and Medal, German Physical Society (DPG), Germany, and Institute of Physics (IOP), London, UK
- since 2016 Member, Academia Europaea
- 2016 Gold Medal, Spanish Royal Physics Society, Spain
- since 2014 Foreign Associate Member, National Academy of Sciences (NAS), USA
- 2014 Premio Jaime I de Investigación Básica, Spain
- 2010 Fellow, American Association for Advanced Science (AAAS), USA
- 2004 Member, American Physical Society (APS), USA

### **Research Priorities**

Angel Rubio is a Spanish physicist. He develops theoretical instruments that both aid in the study of electronical reactions of materials and molecules as well as in the prediction of non-equilibrium phases of matter. He is known for his highly impactful works and leadership in computational solid-state physics, predicting novel materials properties at the nanometer scale, and, more recently, new non-equilibrium phases of matter, opening the fields of cavity materials engineering and QED-

polaritonic chemistry. He is considered a pioneer of computer-aided material science and is one of the founders of modern theoretical spectroscopy.

Angel Rubio research focuses on the modelling and theory of the electronic and structural properties of condensed matter. He develops theoretical instruments that underpin the study of electronic reactions of materials and molecules as well as the prediction of non-equilibrium phases of matter. He is considered a pioneer of computer-aided material science and is one of the founders of modern theoretical spectroscopy. The instruments he developed make it possible to calculate the electronic excitation of materials and nanostructures. Rubio and his group are the originators and developers of the widely used ab initio computational materials research open-source project octopus (<http://www.tddft.org>) that simulates the non-equilibrium dynamics of quantum matter under the influence of arbitrary time-dependent fields.

Rubio's findings on computational solid-state physics embrace the modification of the molecular chemical landscape and reactivity by coupling molecules to quantum cavity vacuum fluctuations (polaritonic chemistry). He developed and established the theoretical framework for "Quantum-Electrodynamic Density Functional Theory (QEDFT)". This theory is used to describe strong light-matter phenomena in chemistry and material science. It is a generalisation of time-dependent Density Functional Theory (DFT) that explicitly treats time-dependent interactions of protons and electrons. His theories provide novel insights on the changes of the molecular chemical landscape and its reactivity by coupling molecules to vacuum fluctuations in quantum cavities. This allows for the prediction and description of newly emerging material states.

Angel Rubio also accomplished breakthrough work on composite nanotubes, new light-driven collective phenomena in solids, theoretical spectroscopy and its applications to quantum materials, Floquet and cavity materials engineering and moiré quantum simulators. He worked on the theory of the electronic structure of low-dimensional systems, molecular compounds, and clusters – most notably of carbon and boron-carbon-nitrogen nanostructures.