## CURRICULUM VITÆ PERSONAL INFORMATION

Name:	Jenny G. Vitillo
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# **EDUCATION**

2005 **Ph.D. in Materials Science and Technology**, University of Turin, Italy.

Academic discipline: Materials for *hydrogen storage*. Thesis Title: "A theoretical and experimental study of molecular interactions involved in hydrogen storage in porous materials". Scientific Supervisor: Prof. <u>G. Ricchiardi</u>.

2002 **M.S. in Materials Science** with 110/110 cum laude, mention, and dignity of publication, University of Turin, Italy.

Academic discipline: *Heterogeneous catalysis*. Thesis Title: "Quantum mechanical modelization of Cr(II) sites on silica active in the ethylene polymerization". Scientific Supervisor: Prof. C. Lamberti.

# **CURRENT AND PAST POSITIONS**

- 2021-today Associate professor, University of Insubria, Como, Italy.
- 2023 Scientific Italian Qualification/Habilitation for the participation to the selections for full professor positions in the sectors 03/A2 (Physical Chemistry), 03/B1 (Inorganic Chemistry), 03/B2 (Materials Engineering) (ASN2022).
- 2022 Visiting scholar, University of Chicago, IL (MOFs for electrocatalysis, prof. L. Gagliardi, prof. J. S. Anderson).
- 2018-2021 Assistant professor (RTDB), University of Insubria, Como, Italy.
- 2017-2018 Postdoctoral fellowship, Department of Chemistry, University of Minnesota, MN (prof. L. Gagliardi, prof. C. C. Lu).
- 2016-2017 Postdoctoral fellowship, Department of Chemistry, University of Turin, Italy
- 2015 Visiting Scholar, UC Berkeley, CA (MOFs synthesis, prof. J.R. Long).
- 2013-2016 Postdoctoral fellowship, Department of Science and High Technology, University of Insubria, Como, Italy. Fund for investment in basic research (Impact project, <u>FIRB 2012</u>).
- 2005-2013 Postdoctoral fellowship, Department of Chemistry, University of Turin, Italy.

# EXPERTISE AND KNOWLEDGE

Jenny G. Vitillo is an expert in energetic and environmental relevant challenges, in particular hydrogen storage, light harvesting, and carbon dioxide capture, utilization and storage (CCUS), and the catalytic conversion of alkane to alcohols. She has exploited almost all the characterization techniques that are relevant in Materials Science both on the computational (quantum mechanics – DFT and multireference wave function methods – and molecular mechanics) and experimental (volumetry, gravimetry, microcalorimetry, powder X-ray diffraction, scanning electron microscopy, differential scanning calorimetry, thermogravimetry, mass spectroscopy, IR, UV-visible and photoluminescence spectroscopies) points of view, focusing on investigating materials for catalysis, energy (storage and delivery), and gas storage and separation. Experience as experimentalist for X-ray absorption and diffraction measurements in large scale facilities (ESRF, BESSY-II). She is also expert in materials synthesis, in particular of metal organic frameworks (MOFs), metal oxides, metal nanoparticles, and organometallic compounds in the air and in inert atmosphere.

# **PUBLICATION RECORD**

From Web of Science (November 2022): **96** publications in peer-reviewed journals (26 as first author and 24 as corresponding author); **2** book chapter; **4757** ISI-citations (without self-citations); *h-index* = **36**.

About 160 contributions to national and international congresses. Participation to 68 national and international congresses. JGV has provided **26** oral communications, 20 in international (2 invited presentation, 3 invited key-note lectures) and 6 in national (2 invited) congresses, schools, and workshop. She has also delivered > 30 invited presentations as part of project meetings in different universities, research centers, and companies. Chairman in three international congresses. Member of the Organizing Committees of an international workshop, of ET14 symposium "Materials Science Facing Global Warming—Practical Solutions for Our Future" for the 2018 MRS Fall Meeting and Exhibit (Leader) and of the panel "Materials Needs for Energy

Sustainability by 2050" for the 2018 MRS Fall Meeting and Exhibit. Member of the Organizer Committee for the "NIS colloquium. Harnessing the Power of Light in Hybrid Materials" (Torino, Italy, 2016). Lead organizer and speaker of the annual "Global Women's Breakfast" for IUPAC100 in Como in 2019, and for IUPAC in 2020, 2022, and 2023. Organizing committee member and speaker for the "Le umaniste incontrano le scienziate" conference for the UNESCO Chair on Gender Equality of the University of Insubria in 2023. Guest editor for the special issue of Chem. Rev. "Carbon Capture and Separation" (2017). Member of the Editorial Board for DOE EFRC newsletter in 2017-2018. Review editor of "Frontiers in Energy Research", for the section "Carbon Capture, Storage, and Utilization". Editorial Board Member of "Applied Sciences" since 2019 (MDPI journals). Presently, she is Guest Editor the special issue "Hybrid Pores for CO<sub>2</sub> Technologies" for Materials Advances.

## FUNDING ID

#### (participated in or leader of the following recent research projects)

#### DOE funding

- 2022-today Catalyst Design for Decarbonization Center (CD4DC, Energy Frontier Research Center, US DOE funds, DE-SC0023383). <u>Collaborator</u> (36 months).
- 2017-2022 Inorganometallic Catalyst Design Center (ICDC, Energy Frontier Research Center, US DOE funds, DE-SC0012702). <u>Scientific Coordinator (12 months), Participant</u>. Funding to the Consortium: 12 M\$
- 2017-2019 Nanoporous Materials Genome Center (NMGC, Materials Genome Initiative, US DOE funds). <u>Participant</u>.

#### Recent EU funding

- 2022-2023 RSC Research Fund grant (R21-5866640195). Funding: 4.5k€. Synthesis and catalysis of Cubased materials. Funding agency: Royal Society of Chemistry. <u>Principal Investigator.</u>
- Proposal CH6251 at ESRF, Grenoble (France), "Local structural and chemical characterization of self-healing copper nanoparticles as catalyst for pharmaceutical and energy applications". As the overall cost of 1 h measurement at synchrotron sources is evaluated between 1 and 2 k€/h, the 72 h experiment corresponds to a funding of the research roughly evaluated between 72 and 144 k€. Main Proposer.
- 2013-2016 VII EU-Framework Program: "Advanced Materials and Electric Swing Adsorption Process for CO<sub>2</sub> Capture", Project ID: 608534 Advanced (MATESA). <u>Participant.</u> Funding to the Turin unit: 354 k€
- 2013-2016 European COST programme, COST Action MP1202: HINT (Rational design of hybrid organic-inorganic interfaces: the next step towards advanced functional materials). <u>Participant.</u>
- 2012-2014 FCH JU platform (Fuel Cells and Hydrogen Joint Undertaking) entitled "Novel H<sub>2</sub> storage materials for stationary and portable applications" (Bor4Store). <u>Participant</u>. Funding to the Turin unit: 242 k€
- 2012 Proposal CH3566 at ESRF, Grenoble (France), "Investigation of the photo-chromic chemical behaviour of Ti-based metal-organic (MOF) and organic-inorganic compounds by means of hard photon-in photon-out spectroscopy". As the overall cost of 1 h measurement at synchrotron sources is evaluated between 1 and 2 k€/h, the 72 h experiment corresponds to a funding of the research roughly evaluated between 72 and 144 k€. <u>Main Proposer</u>.
- 2009-2013 VII EU-Framework Program, NMP-2008-2.4-1: Inorganic-Organic Hybrid Materials. "Nanoporous Metal-Organic Frameworks for production" (NANOMOF). <u>Participant</u>. Funding to the Turin unit: 259 k€
- 2012-2015 VII EU-Framework Program, FCH JU platform (Fuel Cells and Hydrogen Joint Undertaking), "Fuel Cell Coupled Solid State Hydrogen Storage Tank" (SSH2S). <u>Participant.</u> Funding to the Turin unit: 430 k€
- 2006-2009 NMP-4: "Functional Metal Organic Framework as Heterogeneous Catalysts" (MOFCAT). <u>Participant</u>. Funding to the Turin unit: 377 k€
- 2005-2010 NMP3-CT-2005: "Integrated Design of Catalytic Nanomaterials for a Sustainable Production" (IDECAT). <u>Participant</u>. Funding to the Turin unit: 100 k€

Recent funding from other international agencies

2022-2023 RSC Research Fund grant (R21-5866640195). Funding: 4.5k€. Synthesis and catalysis of Cubased materials. Funding agency: Royal Society of Chemistry. <u>Principal Investigator.</u>

# Recent national and regional funding

- 2013-2016 FIRB 2012 PROGRAMMA "FUTURO IN RICERCA" "ImPACT: Impose Pressure And Change Technology Nanostructured systems confined in zeolitic supports". <u>Unit Coordinator.</u> Funding to the University of Insubria unit: 307 k€. Systems developed and studied: dyes encapsulated in porous substrates for light harvesting.
- 2012-2015 PRIN 2010-2011 "Mechanisms of CO<sub>2</sub> activation for the design of new materials for energy and resource efficiency". <u>Participant.</u> Funding to the Turin unit: 140 k€.

Internal competitive calls

- 2021 Grant for the international mobility of faculty members for the 2020/2021 academic year Funding agency: Università dell'Insubria. 2500 €
- 2021 Grant for the funding of a research assistant position. Funding agency: Università dell'Insubria
  23786 €
- 2020 Grant for the international mobility of faculty members for the 2019/2020 academic year Funding agency: Università dell'Insubria. 2500 €

# MAJOR COLLABORATIONS

University of Chicago (prof. L. Gagliardi) [modeling, design and synthesis of catalysts based on metal organic frameworks]

University of Minnesota (prof. A. Bhan) [modeling, design and synthesis of catalysts based on metal organic frameworks]

University of Bonn (prof. C. C. Lu) [modeling, design and synthesis of catalysts based on metal organic frameworks]

Ecole Polytechnique Fédérale de Lausanne, Sion, Switzerland (prof. B. Smit, C. P. Ireland)

University of Stavanger, Norway (Prof. O. Zavorotynska) [complex hydrides]

IFE, Kjellar, Norway (Dr. B. Hauback, Dr. S. Deledda, Dr. C. Frommen) [complex hydrides]

Chennai Institute of Technology, India (prof. J. Ethiraj) [3D printing]

University of Nottingham, UK (prof. A. Laybourn) [MOFs]

LUMS, Pakistan (prof. Muhammad Zaheer) [MOFs]

Università dell'Insubria, Como (prof. E. Fois, Dr. G. Tabacchi) [light harvesting], (prof. A. Maspero) [hydrogenation reactions]

This map shows the world distribution of co-authors in JGV publications.



#### **REVIEWER ACTIVITY**

- **Conferences** Member of the Review Panel of the 2016 Global Conference on Polymer and Composite Materials (PCM2016, May 20-23, 2016, Hangzhou, China).
- **Projects** EU COST Association, the French National Research Agency (ANR), the German Academic Exchange Service (DAAD), King Fahd University of Petroleum & Minerals (Saudi Arabia), the Poland National Science Center, and the Swiss National Science Foundation (SNSF).
- Journals Nature Chem., Nature Commun., Chem, Chem Catalysis, Coord. Chem. Rev., J. Amer. Chem Soc., JACS Au, Angewandte Chemie, J. Mater. Chem. C, ACS Sustainable Chemistry & Engineering, Chem. Sci, Chem. Soc. Rev., ACS Catal., ACS Appl. Mater. Inter., ChemSusChem, Inorganic Chemistry, Chemical Communications, Journal of Catalysis, J. CO<sub>2</sub> Utilization, ACS Applied Nano Materials, Journal of Physical Chemistry C, International Journal of Hydrogen Energy, Physical Chemistry Chemical Physics, International Journal of Applied Ceramic Technology, Journal of Alloys and Compounds, Industrial & Engineering Chemistry Research, Molecules, Frontiers in Energy Research, ChemistrySelect, Green Processing and Synthesis and Computational and Theoretical Chemistry.

## **RESEARCH MENTORSHIP**

- 2022-today Supervisor of 1 master thesis student at the University of Insubria, Italy.
- 2021-today Advisor of 1 Postdoctoral Researcher at the University of Insubria, Italy.
- 2013-2016 Co-supervisor of 1 doctoral student at the University of Turin, Italy (employed in R&D in Luxottica)
- 2005-2017 Co-supervisor of 2 master students and 3 bachelor students at the University of Turin. Of them, 1 continued as a PhD student at University of Turin, 1 is a researcher at Argotec, Turin (PP), 1 is employed by industry (Prototipo Technologies Srl, PP) 1 opened what it is now a famous bakery in Turin.
- 2003-today Tutor for undergraduate and graduate students and Post Doc researchers in their research activities.

# **TEACHING ACTIVITIES**

- 2023 Vibrational and electronic spectroscopies for the characterization of Metal-Organic Frameworks (Ph.D. in Chemical and Environmental Sciences), University of Insubria, Italy (12 h, 3 credits).
- 2022 Vocational guidance in the High Schools for Chemistry (front lessons and laboratory), University of Insubria, Italy (4 h).
- 2021-today Materials for energy (MS in Chemistry and Industrial Chemistry), University of Insubria, Italy (64 h, 8 credits).
- 2020-today Molecular Spectroscopy (MS in Chemistry and Industrial Chemistry), University of Insubria, Italy (64 h, 8 credits).
- 2018-2020 Molecular Spectroscopy (MS in Chemistry, Industrial Chemistry and Physics), University of Insubria, Italy (72 h, 8 credits).
- 2016 Volumetry module, Materials for Energy Laboratory (bachelor in Materials Science and Technology), University of Turin, Italy.
- 2015 Volumetry module, Materials for Energy Laboratory (bachelor in Materials Science and Technology), University of Turin, Italy.
- 2011 Introduction to volumetry module, Physical Chemistry (MS in Materials Science and Mamaself master), University of Turin, Italy.
- 2010 Spectroscopy module, Spectroscopic methods and Microscopies (bachelor in Materials Science), University of Turin, Italy.
- 2009-2014 Tutor for the Stage in a University Laboratory (vocational guidance in the High Schools for the Materials Science), University of Turin, Italy.
- 2009 Theoretical lab module, Chemical bond and Spectroscopy (BS in Industrial Chemistry), University of Turin, Italy.
- 2007-2010 Physical chemistry laboratory (BS in Materials Science, lab assistant), University of Turin, Italy.
- 2007 Computer science for the chemistry (BS in Advanced Chemical Methodologies, lab assistant), University of Turin, Italy.

2007 General chemistry laboratory (BS in Industrial Chemistry, lab assistant), University of Turin, Italy.

2006-2007 Basics of materials science (vocational guidance in the High Schools for the Materials Science), University of Turin, Italy.

## INSTITUTIONAL RESPONSABILITIES

(2018-today) Faculty member of the course board for the degree in Chemistry, University of Insubria, Como, Italy.

(2018-2020) Faculty member of the course board for the degree in Physics, University of Insubria, Como, Italy.

(2022-today) Faculty member of the board for the Ph.D degree in Chemical and Environmental Sciences DISCA, University of Insubria, Como, Italy.

(2019/10/04, 2021/08/07) PhD thesis committee member: Ecole Polytechnique Fédérale de Lausanne (EPFL), Sion, Switzerland.

(2019/02, 2019/12, 2020/12, 2021/06, 2022/03, 2022/06, 2022/12, 2023/02/21, 2023/03/21) MS and BS thesis committee member: University of Insubria, Como, Italy.

(2021/07/21) President of the Faculty committee for the selection of postdoctoral researchers: University of Insubria, Como, Italy.

(2022/07) Committee member for patent approval, University of Insubria, Italy.

(2008, 2013) Committee member for instrument acquisition though tender: University of Torino, Italy.

## CURRENT MEMBERSHIP IN PROFESSIONAL ORGANIZATIONS

American Chemical Society, Royal Society of Chemistry (MRSC).

## **TRACK-RECORD**

In the period 2005-2023, Jenny G. Vitillo has published 96 papers in international peer-reviewed journals. Among top journals of different disciplines: (a) Chemistry: Chem. Rev. (1), J. Am. Chem. Soc. (4), Nature Commun. (1), ChemSusChem (3), Chem. Comm. (1), Mater. Chem. Front. (1), Appl. Catal. B: Environm. (1), J. Phys. Chem. C (14), Langmuir (1), Phys. Chem. Chem. Phys. (14), Dalton Trans. (4), J. Phys. Chem. B (1), J. Phys. Chem. A (2), Energies (1); (b) Catalysis: ACS Catal (2), Catal. Today (2); (c) Materials Science: Adv. Mater. (1), Chem. Mater. (8), J. Mater. Chem. A (1), Inorg. Chem. (2), RSC Adv. (2), ACS Appl. Mater. Interfaces (2), Macromolecules, Int. J. Hydrogen En. (4), Carbon (1), J. Alloy. Compd. (2); (d) Earth Science: Eur. J. Mineral. (1), Appl. Geochem. (1).



Results found103Sum of the times cited5005without self-citations4750Average citations per item48.59h-index36

## **REPRESENTATIVE PUBLICATIONS OF THE SCIENTIFIC PRODUCTION**

Citation numbers are from the Web of Science:

Refs. [1-3] and [7] represent examples of studies on hydrogen storage in microporous materials and in complex hydrides, respectively. Ref. [1] is a pure theoretical article, clearly demonstrating the inadequacy of zeolites (since then a material class often indicated as possible candidate for this purpose) as H<sub>2</sub> storage materials for the automotive sector. Refs. [2,3] are two among the most cited articles in this field showing a combined theoretical, volumetric and spectroscopic approach to the study of hydrogen interaction with materials. Ref. [7] shows the same hybrid approach to the study of the dehydrogenation of a complex hydride,  $\gamma$ -Mg(BH<sub>4</sub>)<sub>2</sub>, reporting significant advances in the understanding of this process. Ref. [4] reports an example of theoretical study on materials for CO<sub>2</sub> separation and storage. Ref. [8] is an invited review on the CO<sub>2</sub> adsorption,

separation, recycling and storage, testifying the international recognized leadership in this field. Ref. [5] reports on a relevant example of dye molecules self-assembled in microporous materials for light harvesting. Ref. [8] uses an experimental multi-technique approach to determine and characterize the CCS performances of UTSA-16. Ref. [9,10] is a study employing DFT and multireference wave function-based methods to tackle the difficult task of the modeling a high spin Fe-based catalyst for the C-H bond activation of methane to methanol and ethane to ethanol.

- 1. J. G. Vitillo, G. Ricchiardi, G. Spoto, and A. Zecchina, "Theoretical maximal storage of hydrogen in zeolitic frameworks", *PCCP*, **7**, 3948 (2005). **Times cited: 85**.
- 2. A. Zecchina, S. Bordiga, J. G. Vitillo, G. Ricchiardi, C. Lamberti, G. Spoto, M. Bjørgen and K.P. Lillerud, "Liquid Hydrogen in Protonic Chabazite", *J. Am. Chem. Soc.*, **127**, 6361 (2005). **Times cited: 185.**
- J. G. Vitillo, L. Regli, S. Chavan, G. Ricchiardi, G. Spoto, P. D. C. Dietzel, S. Bordiga, and A. Zecchina, "Role of exposed metal sites in hydrogen storage in MOFs", *J. Am. Chem. Soc.* 130, 8386 (2008). Times cited: 332.
- 4. [\*] J. G. Vitillo, M. Savonnet, G. Ricchiardi and S. Bordiga, "Tailoring MOFs for CO<sub>2</sub> capture: the aminoeffect", *Chem. Sus. Chem.*, **4**, 1281 (2011). **Times cited: 52.**
- 5. L. Gigli, R. Arletti, G. Tabacchi, E. Fois, J.G. Vitillo, G. Martra, G. Agostini, S. Quartieri, G. Vezzalini, "Close-Packed Dye Molecules in Zeolite Channels Self Assemble into Supramolecular Nanoladders", *J. Phys. Chem. C* 2014-033564 (2014). **Times cited: 36.**
- 6. [\*] J. G. Vitillo, "Magnesium-based systems for carbon dioxide capture, storage and recycling: from leaves to synthetic nanostructured materials", *RSC Adv.*, **5**, 36192 36239 (2015). **Times cited: 45.**
- [\*] J. G. Vitillo, S. Bordiga, M. Baricco, "Spectroscopic and structural characterization of thermal decomposition of γ-Mg(BH<sub>4</sub>)<sub>2</sub>: dynamic vacuum vs. H<sub>2</sub> atmosphere", *J. Phys. Chem. C*, **119**, 25340–25351 (2015). Times cited: **20**.
- A. Masala<sup>†</sup>, J. G. Vitillo<sup>†</sup>, G. Mondino, C. A. Grande, R. Blom, M. Manzoli, M. Marshall and S. Bordiga, "CO<sub>2</sub> capture in dry and wet conditions in UTSA-16 metal organic framework", ACS Appl. Mater. Interfaces, 9, 455–463 (2017). Times cited: 34.
- 9. [\*] J. G. Vitillo, A. Bhan, C. J. Cramer, C. C. Lu, L. Gagliardi, "Quantum Chemical Characterization of Structural Single Fe(II) Sites in MIL-Type Metal–Organic Frameworks for the Oxidation of Methane to Methanol and Ethane to Ethanol.", *ACS Catal.*, **9**, 2870-2879 (2019). **Times cited: 39**.
- [\*] J. G. Vitillo, C. C. Lu, C. J. Cramer, A. Bhan, L. Gagliardi, "Influence of First and Second Coordination Environment on Structural Fe(II) Sites in MIL-101 for C–H Bond Activation in Methane", ACS Catal., 11, 579–589 (2021). Times cited: 10.

# INVITED PRESENTATIONS TO PEER-REVIEWED, INTERNATIONALLY ESTABLISHED CONFERENCES

- 2023 "Carbon capture, utilization, and storage for an optimized-cost 1.5 °C-committed pathway: the implementation at the global and the atomistic scale", J. G. Vitillo, ACS Spring 2023, PHYS symposium "Carbon Separation and Capture at the Atomistic Level: Theory and Experiment" Indianapolis, IN (March 26 30, 2023).
- 2022 "The importance of phase change in materials for hydrogen separation and storage" (keynote), J. G. Vitillo, MSSC2022 Ab initio Modelling in Solid State Chemistry, London (UK) (September 19-23, 2022).
- 2018 "Materials Science Facing Global Warming—So What?" (keynote) J. G. Vitillo; "2018 MRS Fall Meeting and Exhibit", Boston MA (November 25-30, 2018).
- 2014 "Carbon dioxide capture and recycling in microporous materials" (keynote), J. G. Vitillo, J. Ethiraj, F. Giordanino, V. Crocellà, G. Ricchiardi, E. Groppo, M. Baricco, F. Bonino, S. Chavan, S. Bordiga, "Advanced Functional Materials", Nessebar, Bulgaria (September 3-6, 2014).
- 2013 "Enhancing CCS performances of microporous materials by basic oxide coating" J. G. Vitillo, F. Giordanino, G. Ricchiardi, V. Crocellà, S. Bordiga, "NIS Colloquium: Advances in CO<sub>2</sub> capture and reactivity with new materials", Torino, Italy (November 15<sup>th</sup>, 2013).
- 2013 "Design of hydrogen storage materials: A multitechnical approach" (keynote), J. G. Vitillo, "Materials for Clean Energy and Optics workshop", Pravets, Bulgaria (April 4-7, 2013).
- 2010 "Tailoring MOFs for CO<sub>2</sub> storage: the amino-effect", J. G. Vitillo, S. Chavan, B. Seyyedi, F. Bonino, D. Farrusseng, S. Bordiga, "Computational Carbon Capture" workshop, Lausanne, Switzerland CECAM-HQ-EPFL (July 26-28, 2010).
- 2008 "CH<sub>4</sub> storage in microporous materials", J. G. Vitillo, "NIS Colloquium: H<sub>2</sub>, CH<sub>4</sub> and CO<sub>2</sub>: separation, storage and activation", ENI Ist. Guido Donegani, Novara, Italy (May 27th, 2008).