PERSONAL INFORMATION

Dario Duca

viale delle Scienze, Ed.17, Palermo, 90128 Italy

+39-091-23897975

https://www.unipa.it/persone/docenti/d/dario.duca

Enterprise	University	EPR
☐ Management Level	☒ Full professor	☐ Research Director and 1st level Technologist / First Researcher and 2nd level Technologist
☐ Mid-Management Level	☐ Associate Professor	☐ Level III Researcher and Technologist
☐ Employee / worker level	☐ Researcher and Technologist of IV, V, VI and VII level / Technical collaborator	☐ Researcher and Technologist of IV, V, VI and VII level / Technical collaborator

WORK EXPERIENCE

2001 – present Full Professor of General and Inorganic Chemistry at the University of Palermo.
1998 – 2001 Associate Professor of General and Inorganic Chemistry at the University of Salerno.
1993 – 1998 Italian Council of National Research (CNR) researcher at the Institute of Chemistry and Technology of the Natural Products (ICTPN) and member of its Scientific Council.
1992 – 1993 Research associate fellow at ICTPN-CNR granted by PUMEX s/a of Lipari.

Activities along the work experience:

- Visiting Scientist at the Hungarian Academy of Sciences, KKKI-MTA, IKI-KFKI-MTA, (1994 – 1997).
- Head of the Council of the Conservation and Valorization of Biodiversity Degree Course at the Science Faculty of the University of Palermo (2001 – 2002).
- Editor for the Italian translation of the fourth edition of the text: “Inorganic Chemistry”, authors G. L. Miessler and D. A. Tarr, for the Piccin Nuova Libraria of Padua (2011) and of the fourth edition of the text: “Descriptive Inorganic Chemistry”, authors G. Rayner-Canham and T. Overton, for the EdiSES of Naples (2017).
- Italian Project Coordinator and Member of the Steering Committee of i) NanoCat (STREP, 6th Framework Program of the European Community, NMP-2002-3.4.1.1-1, 2005 – 2008); ii) POLYCAT (LSICP, 7th Framework Program of the European Community, NMP-2009-3.2-1, 2010 – 2014); SusFuelCat (SSICP, 7th Framework Program of the European Community, NMP.2012.1.1-1, 2013 – 2017).
- Collaborator and local responsible of national project, *e.g.* MiSE-CNR project Storage systems, including electrochemical and power to gas, and related interfaces with the networks, located within the PTR 2019-2021 of the Research of the National Electricity System (RdS) presented by the CNR.
- Teacher of General and Inorganic Chemistry courses and member of Doctoral Schools.
- Developer of i) Size Exclusion Chromatography (SEC) methods and of the related algorithms to study catalytic support properties; ii) the first kinetic time-dependent Monte Carlo algorithms to study big-bang and steady-state surface events and catalysis; iii) deterministic, vectorial and stochastic algorithms to analyse at atomistic level heterogeneous catalysis processes; iv) graphic software to study surface process; v) conformational space analysis algorithms.
- Head of the Computational Chemistry for Catalytic Processes (CCCP) group.
- Reviewer of national and international research projects and scientific papers.

EDUCATION AND TRAINING

1990 – 1992 Sc.D. fellowship, working on heterogeneous catalysis, granted by the Italian CNR.
1988 – 1990 Ph.D. courses in Chemical Sciences, granted by the Ministry of University.
1986 Graduated, cum laude, in Chemistry at the University of Palermo and achievement of the professional qualification to the activity of Chemist.

In these periods contributed to the:

- investigation of the: i) structure and activity of organometallic species having biological interest and ii) catalytic materials by TEM, SAXS, WAXS and XPS methods.

While developed:

- i) titration methods employing IR, NMR and Mössbauer spectroscopies to study structure/bio-activity correlations in organotin species; ii) synthesis methods to obtain supported catalysts involving different support and metals; iii) algorithms to model SAXS and WAXS data of materials of potential catalytic use.

PERSONAL SKILLS

Mother tongue(s) Italian

Other language(s) English: proficient user

Job-related skills Research-group leadership and coordination experience, project management.

Digital skills Proficiency in Fortran, C-Lisp, LaTeX, HTML, CSS, perfect command of Linux, macOS and Windows codes, Google tools, use of email and shared workspace services, development and use of chemical representation and calculation codes.

Other skills Attention to detail, focus, time management, high tolerance of change, uncertainty, good at working and pressure, adaptability, strong work ethic, reliability, excellent communication skills and problem-solving abilities, critical thinking, conflict management skills.

ADDITIONAL INFORMATION

Selection of Recent Publications

1) Cortese, R., Sifontes Herrera, V. A., Duca, D., Murzin, D. Yu. “L-Arabinose conformers adsorption on ruthenium surfaces: a DFT study” J. Phys. Chem. C, 116, 14908–14916 (2012) – doi:10.1021/jp3026336.
2) Prestianni, A., Ferrante, F., Simakova, O.A., Duca, D., Murzin, D.Yu.,“Oxygen-Assisted Hydroxymatairesinol Dehydrogenation: A Selective Secondary-Alcohol Oxidation over a Gold Catalyst” Chem. Eur. J, 19 (14), 4577–4585 (2013) – doi: 10.1002/chem.201202957.
3) Prestianni, A., Crespo-Quesada, M., Cortese, R., Ferrante, F., Kiwi-Minsker, L., Duca, D.,“Structure Sensitivity of 2-methyl-3-butyn-2-ol Hydrogenation on Pd: Computational and Experimental Modeling” J. Chem. Phys. C, 118 (6), 3119–3128 (2014) – doi: 10.1021/jp4114859.
4) Prestianni, A., Ferrante, F., Sulman, M.E., Duca, D., “DFT Investigation on the Nucleation and Growth of Small Palladium Clusters on a Hypercrosslinked Polystyrene Matrix” J. Chem. Phys. C, 118 (36), 21006–21013 (2014) – doi: 10.1021/jp506320z.
5) Crespo-Quesada, M., Yoon ,S., Jin, M., Prestianni, A., Cortese, R., Cárdenas-Lizana, F., Duca, D., Weidenkaff, A., Kiwi-Minsker, L., “Shape-Dependence of Pd Nanocrystal Carburization during Acetylene Hydrogenation” J. Chem. Phys. C, 119 (2), 1101–1107 (2015) – doi: 10.1021/jp510347r.
6) Cortese, R., Ferrante, F., Roggan, S., Duca, D., “N-Doped Carbon Networks: Alternative Materials Tracing New Routes for Activating Molecular Hydrogen” Chem. Eur. J, 21, 3806–3814 (2015) – doi: 10.1002/chem.201405896.
7) Schimmenti, R., Cortese, R., Duca, D., Mavrikakis, M., “Boron Nitride-supported Sub-nanometer Pd6 Clusters for Formic Acid Decomposition: A DFT Study” ChemCatChem. 9, 1610−1620 (2017) – doi: 10.1002/cctc.201700619.
8) Schimmenti, R., Cortese, R., Godina, L., Prestianni, A., Ferrante, F., Duca, D., Murzin, D. Yu., “A Combined Theoretical and Experimental Approach for Platinum Catalyzed 1,2-Propanediol Aqueous Phase Reforming” J. Phys. Chem. C. 121(27), 14636–14648 (2017) – doi: 10.1021/acs.jpcc.7b03716.
9) Koichumanova, K., Vikla, A. K. K., Cortese, R., Ferrante, F., Seshan, K., Duca, D., Lefferts, L., “In Situ ATR-IR Studies in Aqueous Phase Reforming of Hydroxyacetone on Pt/ZrO2 and Pt/AlO(OH) Catalysts: The Role of Aldol Condensation” Appl. Catal. B Environ. 232, 454–463 (2018) – doi: /10.1016/j.apcatb.2018.03.090.
10) Arena F., Ferrante F., Di Chio R., Bonura G., Frusteri F., Frusteri L., Prestianni A., Morandi S., Martra G., Duca D., “DFT and kinetic evidences of the preferential CO oxidation pattern of manganese dioxide catalysts in hydrogen stream (PROX)” Appl. Cat. B: Env. 300, 120715 (2022) – doi: 10.1016/j.apcatb.2021.120715.