# Curriculum Vitae (Prof. Daniel Escudero)

# • Short CV

**PERSONAL INFORMATION** Family name, First name: Escudero, Daniel Researcher unique identifier(s): https://orcid.org/0000-0002-1777-8578 / http://scholar.google.es/citations?hl=es&user=SPst3qEAAAAJ

URL for web site: <a href="https://chem.kuleuven.be/en/research/qcpc/cpc/">https://chem.kuleuven.be/en/research/qcpc/cpc/</a>

#### • EDUCATION:

- 2011 **Doctor** rerum naturalium (Dr. rer. nat.) by the **Friedrich-Schiller-Universität** (FSU), Jena, **Germany**. PhD Thesis title: "Spectroscopy and Photochemistry of Transition Metal Complexes: A Quantum Chemical Study". PhD supervisor: Prof. Dr. Leticia González. **Grade: "Summa Cum Laude"**
- 2007 Graduated in Chemistry (Licenciado) by the University of the Balearic Islands (UIB), Spain. Major: Organic Physical Chemistry. Grade: 97 %

## • CURRENT POSITION(S)

- 2020 Head of the Quantum Chemistry and Physical Chemistry Division at the Chemistry Department at KU Leuven (Belgium)
- 2018 Research Assistant BOFZAP Professor at the Chemistry Department at KU Leuven (Belgium)

## PREVIOUS POSITIONS

- 2016 2018 Marie Sklodowska-Curie Research fellow at CEISAM, Université de Nantes (France). Project: CompOLEDs
- 2014 2016 Postdoctoral researcher. CEISAM, University of Nantes (**France**). Supervisor: Prof. **Denis Jacquemin**
- 2011 2014 Postdoctoral researcher. Max-Planck-Institut für Kohlenforschung (Germany). Supervisor: Prof. Walter Thiel
- 2007 2011 PhD student. Institute of Physical Chemistry Friedrich-Schiller Universität Jena (**Germany**). Supervisor: Prof. Leticia González
- 2006 2007 Undergraduate student. Dept. of Organic Chemistry, UIB (**Spain**). Supervisor: Prof. Antonio Frontera

#### • FELLOWSHIPS

- 2018 Attracting talent program of the Autonomous Community of Madrid (not accepted)
- 2016 2018 Marie Sklodowska-Curie action (H2020-MSCA-IF). Project: CompOLEDs

# SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS

2018 – Current supervisor of **6 PhD students** (Prashant Kumar, Koen Veys, Laura Galleni, Jing Gong, Yixuan Li, Arne Meulemans). Supervisor of 2 **Postdoc** (Mariana T. do Casal, Hung Tan Pham). Regular supervision of numerous MsC and undergraduate students.

#### • TEACHING ACTIVITIES

2018 – Master Courses (Chemistry, TCCM MSc) at the KU Leuven (Belgium)

## • INSTITUTIONAL RESPONSIBILITIES

2020 – Head of the Quantum Chemistry and Physical Chemistry Division at the Chemistry Department at KU Leuven (Belgium)

## • COMMISSIONS OF TRUST

# 2022 Member of the FWO Research Expert Pannel (Chemistry, research projects)

2020 – Member of the Editorial Board of Dyes and Pigments.

2020 Scientific Evaluation for ERC-StG (H2020). External Referee for RSF and SNSF

# • SCIENTIFIC TRACK-RECORD AND BIBLIOMETRIC INFORMATION

- Author of **96 articles** and 2 book chapters (among them 2 Acc. Chem. Res.; 1 Adv. Func. Mater.; 2 Chem. Sci.; 1 Angew. Chem. Int. Ed.; 2 J. Chem. Phys. Lett.; 1 Chem. Mater.; 6 Chem. Eur. J; 4 Phys. Chem. Chem. Phys.; 6 Inorg. Chem.; 2 J. Chem. Theory and Comput.) in international peer-reviewed journals. Complete list of publications: <u>http://lirias.kuleuven.be/cv?Username=U0121765</u>
- > 24 oral contributions (**13 keynote&invited**) in international conferences.
- Total number of citations > 3500 (excluding self-cites). Hirsch (H) index: 34. Ranked among the 2% top researchers in chemical-related fields in the standardized citation metrics author database (DOI: 10.17632/btchxktzyw.3)

## MEMBERSHIPS OF SCIENTIFIC SOCIETIES

2020 – Member of the "European Photochemistry Association"

#### Career breaks: Not applicable

#### Five main publications and/or achievements

1. K. Veys, <u>D. Escudero\*</u>. Anti-Kasha Fluorescence in Molecular Entities: Central Role of Electron– Vibrational Coupling. Acc. Chem. Res., 5, 2698-2707 (2022) (Corresponding author / Cover article) [cit=7] [IF=24.5]. Relevance: We developed theoretical descriptors and computational protocols to predict anti-Kasha fluorescence but also to calculate the higher-lying excited-state lifetimes and quantum yields in a semi-quantitative manner. The developed tools enabled us to re-conceptualize the field of Anti-Kasha fluorescence, highlighting the central role of the electron-vibrational coupling, which enabled us to distinguish among three possible regimes leading to anti-Kasha scenarios. It was highlighted in the cover of Acc. Chem. Res. It is a cornerstone of *PhotoLong.* (https://pubs.acs.org/doi/10.1021/acs.accounts.2c00453?goto=supporting-info)

2. X. Zhang, D. Jacquemin, Q. Peng, Z. Shuai, <u>D. Escudero\*</u>. General Approach To Compute Phosphorescent OLED Efficiency. J. Phys. Chem. C, 122, 6340 (2018) (Corresponding author / "Highly Cited Paper" by ISI Web of Knowledge) [cit=69] [IF=4.2]. Relevance: We report a computational protocol to model the temperature-dependent phosphorescent lifetimes and efficiencies of phosphors. It is another cornerstone of *PhotoLong* (<u>http://bit.ly/2t0ukSN</u>).

3. M. Pérez-Escribano, J. Jankowska, G. Granucci, <u>D. Escudero\*</u>. The radiative surface hopping (RSH) algorithm: Capturing fluorescence events in molecular systems within a semi-classical non-adiabatic molecular dynamics framework. J. Chem. Phys., 158, 124104 (2023) (Corresponding author) [IF=4.3]. Relevance: We report the RSH algorithm, a method to model fluorescence within a NAMD framework. It is the most important cornerstone of *PhotoLong*. (https://aip.scitation.org/doi/10.1063/5.0139516)

4. X. Zhang, M. Ivanov, Z. Wang, M. H. E. Bousquet, X. Liu, Y. Wan, J. Zhao<sup>\*</sup>, A. Barbon, <u>D. Escudero<sup>\*</sup></u>, D. Jacquemin<sup>\*</sup>, M. Fedin<sup>\*</sup>. Confinement of the Triplet States in  $\pi$ -Conjugated BODIPY Dimers Linked with Ethynylene or Butadiynylene Bridges: A Different View on the Effect of Symmetry. **Angew. Chem. Int. Ed.**, 61, e202210419 (**2022**) (Corresponding author) [IF=16.8]. **Relevance:** This contribution exemplifies one of the collaborations with my experimental partners. In this paper we studied the excited state deactivation of multichromophoric BODIPY Dimers from a static viewpoint. The developments proposed in *PhotoLong* will permit the dynamic study of these molecular systems. (https://onlinelibrary.wiley.com/doi/full/10.1002/anie.202210419)

5. H.-H. Kuo, S.Kumar, R. L. Omongos, M. T. do Casal, M. E. Usteri, M. Wörle, <u>D. Escudero\*</u>, C.-J. Shih. Design and Synthesis of Asymmetric Au (III) Complexes Exhibiting Bright Anisotropic Emission for High-Performance Organic Light-Emitting Diodes. **Adv. Opt. Mater.**, DOI: 10.1002/adom.202202519 (**2023**) (Corresponding author) [IF=10.1]. **Relevance:** A representative experimental-computational collaboration of my research lab on Au(III) emitters and their excellent performance for OLEDs devices. (https://onlinelibrary.wiley.com/doi/abs/10.1002/adom.202202519)

## Other scientific output and impact:

## Keynote and invited seminars at international conferences (2020-2023):

(1) "In-silico" Modeling of Fluorescence (Keynote at the APATCC-10 conference, Feb 2023) (2) Anti-Kasha fluorescence: role of the electron-vibrational coupling (PhotoIUPAC conference, Jul 2022) (3) Anti-Kasha emissions: From-First Principles Insights (Keynote at the IC3EM2022 conference, Jun 2022) (4) Benchmarking excited state decay rate theories (EUCO-CC conference, Nov 2021) (5) Anti-Kasha photochemistry: theoretical investigations (Keynote at Computational Photochemistry Online Meeting, Jul 2021) (6) Quantitative determinations of photochemistry from excited state decay rate calculations. Virtual International Seminar on Theoretical Advancements (VISTA) (Vista virtual seminars, Nov 2020)

# List the representative and substantial fellowships, projects and any other kind of research grants you obtained within the five years preceding the submission date of this project application.

- ✓ 2022-2026 Internal Funds KU Leuven (IDN project) with Prof. Taurino, Prof. Janssens, Prof. Deporteere and Prof. Vantomme: 700k€
- ✓ 2022-2025 FWO Junior Research Project (G079122N): 335k€
- ✓ 2021-2024 Internal Funds KU Leuven (IDN project) with Prof. Koeckelberghs and Prof. Molina-López: 700k€
- ✓ 2021-2024 FWO-NAFOSTED (G0E5321N) with Prof. Dehaen and Prof. Nguyen: 340k€
- ✓ 2021-2022 CELSA KU Leuven Funds\_ PhotoSynergy with Dr. Jankowska: 90k€
- ✓ 2018-2021 BOFZAP Research grant (KU Leuven): 100k€
- ✓ MISTI (KU Leuven-MIT) with Prof. Gomez-Bombarelli: 30k€ (2020-2021)
- ✓ FWO-Tournesol with Prof. Jacquemin: 5k€ (2020-2021)
- ✓ Attracting talent program of the Autonomous Community of Madrid: 200k€ (2018)
- ✓ H2020-funding: CompOLEDs, H2020-MSCA-IF-2015 call: 173,076.00€ (2016)