



SEDUTA DEL COLLEGIO DEI DOCENTI DEL 36° CICLO

18 Dicembre 2023

Il Collegio dei Docenti del 36° ciclo del Dottorato di Ricerca in Scienze Fisiche e Chimiche dell'Università di Palermo, regolarmente convocato in modalità telematica dal Coordinatore Prof. Marco Cannas, si riunisce sulla piattaforma Microsoft Teams alle ore 14,30 del giorno 18.12.2023 con il seguente ordine del giorno:

1) Adempimenti dottorandi per l'esame finale di conseguimento del titolo di dottore di ricerca (1° sessione)

2) Varie ed eventuali

Presiede il Coordinatore Prof. Marco Cannas, svolge le funzioni di segretario il Prof. Giuseppe Lazzara

Sono presenti

M. Cannas, A. Pettignano, G. Lazzara, F. Ciccarello, F. Ferrante, G.M. Palma, A. Napoli, , R. Iaria, T. Di Salvo, D. Valenti, S. Agnello, M. Miceli,

Sono assenti giustificati

C. Fazio, F. Reale, S. Milioto, G. Cusumano, S. Miccichè, R. Passante, G. Buscarino, G. Marsella, B. Militello, F. Messina, G. Micela

Sono presenti inoltre i cotutor G. Cavallaro, C. Pinto, S. Lorenzo

Il Presidente, prof. M. Cannas, verificato il numero legale, dichiara aperta la seduta e passa a discutere il primo punto all'ordine del giorno:

1) Adempimenti dottorandi per l'esame finale di conseguimento del titolo di dottore di ricerca

Il presidente illustra gli adempimenti necessari per il conseguimento del titolo di dottore di ricerca per gli allievi del 36° ciclo.

In accordo al cronoprogramma. il presente collegio dei docenti dovrà occuparsi dei seguenti punti:

- formulazione della relazione del dottorando sulle attività svolte
- formulazione del parere per il titolo di Doctor Europaeus
- proposta di formazione delle commissioni giudicatrici
- nomina dei valutatori esterni

per gli allievi che hanno concluso il loro dottorato il 31/10/2023 e intendono sostenere l'esame finale nella seconda sessione (20 febbraio – 3 marzo 2024).



Laura Gueci (Tutor: Prof. Francesco Ferrante; Cotutor: Prof. Dario Duca)

Il collegio prende visione della relazione del dottorando (allegato 1 al verbale).

Il collegio propone che la commissione giudicatrice per l'esame finale sia composta da:

Membri effettivi

- 1) Fabrizio Lo Celso, DiFC, Università degli Studi di Palermo, fabrizio.locelso@unipa.it
- 2) Emilia Sicilia, Università della Calabria
- 3) Antonio Cammarata, Czech Technical University in Prague (Repubblica Ceca)

Membro supplente

Alberto Pettignano, Università degli Studi di Palermo

Il collegio nomina i valutatori esterni:

- 1) Evgeny Pidko Delft University of Technology (Paesi Bassi) e.a.pidko@tudelft.nl
- 2) Ilaria Ciofini, PSL University, Chimie ParisTech (Francia) ilaria.ciofini@chimieparistech.psl.eu

Per l'allieva Laura Gueci, il collegio attesta che sono soddisfatti i criteri per conseguire il titolo di Doctor Europaeus, ed esprime un parere positivo



Alessio Anitra (Tutor: Prof.ssa Tiziana Di Salvo, cotutor: Prof. Rosario Iaria)

Il collegio prende visione della relazione del dottorando (allegato 2 al verbale).

Il collegio propone che la commissione giudicatrice sia composta da:

Membri effettivi

- 1) Marco Miceli, Università degli Studi di Palermo, marco.miceli@unipa.it
- 2) Francesco Tombesi, Università di Roma "Tor Vergata"
- 3) Alessandro Papitto, INAF, INAF-Osservatorio Astronomico di Roma (OAR)

Membro supplente

Costanza Argiroffi , Università degli Studi di Palermo

Il collegio nomina i valutatori esterni:

- 1) Dott.ssa Domitilla De Martino - Astronomo Associato presso l'INAF- Osservatorio Astronomico di Capodimonte Napoli

email: domitilla.demartino@inaf.it

- 2) Dott.ss Sara Elisa Motta - INAF - Osservatorio Astronomico di Brera

email: sara.motta@inaf.it



Yerong Xu (Tutor: Dott. Giancarlo Cusumano; Cotutor: Dott. Ciro Pinto)

Il collegio prende visione della relazione del dottorando (allegato 3 al verbale).

Il collegio propone che la commissione giudicatrice sia composta da:

Membri effettivi

- 1) Marco Miceli, Università degli Studi di Palermo, marco.miceli@unipa.it
- 2) Francesco Tombesi, Università di Roma "Tor Vergata"
- 3) Alessandro Papitto, INAF, INAF-Osservatorio Astronomico di Roma (OAR)

Membro supplente

Costanza Argiroffi, Università degli Studi di Palermo

Il collegio nomina i valutatori esterni:

- 1) Dr. Emanuele Nardini, INAF-Osservatorio Astrofisico di Arcetri, emanuele.nardini@inaf.it
- 2) Dr. Junjie Mao, Tsinghua University, Beijing, China, jmao@tsinghua.edu.cn

2) Varie ed eventuali

Non ci sono varie ed eventuali.

Il verbale è approvato seduta stante. La seduta si chiude alle ore 15:10.

Il Presidente

Prof. Marco Cannas

Il Segretario

Prof. Giuseppe Lazzara



Allegato 1

PHD IN PHYSICAL AND CHEMICAL SCIENCES, XXXVI COURSE

PhD Candidate: Laura Gueci

Transcript of Records

Tutor: Prof. Francesco Ferrante

Cotutor: Prof. Dario Duca

Courses/school/exam scores:

Courses

- “Thermodynamic Techniques for the Characterization of Nanostructured Materials”. Instructor: dott. Giuseppe Cavallaro. 21-25 June 2021. Exam taken.
- “Organic/Inorganic Nanocomposites: Properties and Applications”. Instructor: dott. Giuseppe Cavallaro. 05-09 July 2021. Exam taken.
- “Experimental techniques in astroparticle physics”. Instructor: prof. Giovanni Marsella. 18 February-22 March 2022 (16h). Exam taken.
- “Python programming and quantum physics”. Instructor: prof. Salvatore Lorenzo. 15 March-04 May 2022 (20h).

Schools

- “XIII Scuola di ricerca educativa e didattica chimica Ulderico Segre”, online. Dates: 17-30 November 2021 (14h).
- “ESQC2022: European Summer School in Quantum Chemistry”. Dates: 11-24 September 2022 (80h). Exam taken.

Research and training periods abroad

Abo Akademi University, Turku - Finlandia, from february, 28th 2023 to june, 2nd 2023.
Scientific research about hydrocarbon cracking by means of metal-zeolite bifunctional catalysts. under the supervision of Prof. Dmitry Murzin. This activity was inherent to the PhD project.

Papers published:

Related to the PhD project

- 1) L. Gueci, M. Bertini, C. Nania, F. Ferrante and D. Duca, “DFT Study of Pt Particle Growth inside β -Zeolite Cages”, The Journal of Physical Chemistry C, vol. 127, p. 14765, 2023.



- 2) L. Gucci, F. Ferrante, M. Bertini, C. Nania and D. Duca, "DFT study on zeolites' intrinsic Brønsted acidity: The case of BEA", *Computational Material Science*, vol. 232, p. 112687, 2024.
- 3) L. Gucci, F. Ferrante, M. Bertini, L. Lisuzzo, M. Martinez-Klimov, Z. Vajglova, N. Kumar, D.-Yu. Murzin and D. Duca, "The acid strenght of platinum modified H-Beta zeolites: A combined DFT and pyridine-FTIR investigation", in preparation.

Other ISI papers:

- 4) L. Gucci, F. Ferrante, A. Prestianni, F. Arena, and D. Duca, "Benzyl alcohol to benzaldehyde oxidation on MnO_x clusters: Unraveling atomistic features", *Molecular Catalysis*, vol. 513, p. 111735, 2021.
- 5) L. Gucci, F. Ferrante, A. Prestianni, F. Arena, and D. Duca, "Structural, energetic and kinetic database of catalytic reactions: Benzyl alcohol to benzaldehyde oxidation on MnO_x clusters", *Data in Brief*, vol. 38, p. 107369, 2021.
- 6) C. Nania, M. Bertini, L. Gucci, F. Ferrante and D. Duca, "DFT insights into competing mechanisms of guaiacol hydrodeoxygenation on a platinum cluster", *Physical Chemistry Chemical Physics*, vol. 25, p. 10460, 2023.
- 7) F. Ferrante, M. Bertini, L. Gucci and D. Duca, "Butene Isomerization on Palladium Surfaces: Time-Dependent Monte Carlo Studies", *Industrial & Engineering Chemistry Research*, vol. 62, p. 20608, 2023.
- 8) L. Gucci, F. Arena, S. Todaro, G. Bonura, A. Cajumi, M. Bertini, F. Ferrante, C. Nania and D. Duca, "CO-PROX on MnO_x catalysts: DFT-based microkinetics and experimental macrokinetic approaches" submitted to *Catalysis Today*

Conferences/workshop attended:

- **Talks:**

DCTC2022: Workshop della Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana, "Oxidation functionality of MnO_x catalysts: a DFT study to unveil atomistic features", L. Gucci, F. Ferrante, C. Nania, M. Bertini, D. Duca, Florence (ITA), 8th April 2022.

YourHetCat2022: 1st Forum of Young Researchers on Heterogeneous Catalysis, "Platinum modified Beta zeolite catalysts: a DFT study on metal sites formation and energetics", L. Gucci, F. Ferrante, C. Nania, M. Bertini, D. Duca, Szeged (HUN), 11-13 July 2022.



ICGC2022: 9th IUPAC International Conference on Green Chemistry, "Rational Design of Manganese Dioxide Catalyst for the Preferential Oxidation of CO in Hydrogen Stream: From Theory to Practice", F. Arena, F. Ferrante, L. Gucci, G. Bonura, M. Bertini, S. Todaro, F. Frusteri, C. Nania, D. Duca, Athens (GRE) 5-9 September 2022.

Thesis title:

Computational studies of modified H-Beta zeolites for hydrocarbon catalytic conversion

Abstract:

The β -zeolite's Brønsted acidity has been computationally characterized in terms of the deprotonation energy (DPE) values of 30 topologically distinct acidic sites. DPEs were computed through three different approaches within the DFT framework, namely: an ONIOM embedding scheme, full periodic calculations and a novel cluster method specifically designed to avoid the disadvantages related to the other two approaches. The suggested cluster approach, which avoids the necessity of empirical corrections, is proposed as a suitable tool to correct in an algorithmic way the DPE values resulting from periodic calculations. Density functional theory was employed also to identify the preferential location of platinum atoms inside a β -zeolite model and to study the growth of a minimal cluster. Pt atoms migration through cages was also addressed, by means of a transition state search following the NEB approach. A comparative structural analysis involving different cavities and platinum atom numbers showed that the optimal geometry involving a single platinum atom takes place when the formation of an almost linear O-Pt-O arrangement occurs. The metal-acid interactions in platinum-modified β -zeolite catalysts were explored from both experimental and atomistic perspectives, aiming at shedding light on the complex synergy between these functionalities. Various techniques, including Scanning Electron Microscopy, Energy-Dispersive X-ray Microanalysis, Transmission Electron Microscopy, and Fourier Transform Infrared Spectroscopy, were employed to characterize modified catalysts from H-Beta-38 and H-Beta-300 materials prepared by Evaporation Impregnation and Incipient Wetness. It was observed that, at least according to the atomic-level interaction of a single platinum atom with an inner acidic site, the intrinsic Brønsted acidity variation should go in the opposite direction of what is experimentally observed, suggesting that the acid sites affected by modifications are those on the surface of the zeolite crystallites rather than internal sites within the bulk framework. Finally, a DFT analysis was performed to investigate the transformation of n-2-pentene to iso-2-pentene, as part of a hydroisomerization process occurring on a selected Brønsted acidic site of β -zeolite. The results offer valuable insights into the molecular-level details of this specific hydroisomerization process, allowing to discriminate ephemeral intermediates from transition states.

The PhD Board Dean

Prof. Marco Cannas



Allegato 2

PHD IN PHYSICAL AND CHEMICAL SCIENCES, XXXVI COURSE

PhD Candidate: ALESSIO ANITRA

Transcript of Records

Tutor: PROF. TIZIANA DI SALVO

Cotutor: PROF. ROSARIO IARIA

Courses/school/exam scores:

- Project Management in the scientific - spatial context, G. Micela (Unipa, Dec 2021- Jan 2022)
- MILLISECOND PULSARS: THEORY AND OBSERVATIONS, T. Di Salvo (Unipa, Dec 2021- Feb 2022)
- Astrophysics laboratory of thermal X-ray plasmas, C. Pinto (Unipa, Marzo 2023- Maggio 2023)

Research and training periods abroad

- **26/02/2022-25/09/2022 (7 mesi)** Instituto de Astrofísica de Canarias, La Laguna, Santa Cruz de Tenerife, Spain. Tutor: Dr. Teo Munoz-Darias

Conferences/workshop attended:

1. 04/10/2021 – 08/10/2021
Third National Workshop on the SKA Project - The Italian Route to the SKAO Revolution
2. 20/09/2021 – 24/09/2021 – Cagliari, Italia
The 9th Microquasar Workshop: Celebrating over 50 years of discovery.
3. 27/09/2022 – 30/09/2022 – Cefalù (Palermo)
Congresso Nazionale Oggetti Compatti XII Membro del Local Organizing Committee
4. 10/05/2021 – 14/05/2021
NICER Data Analysis and Science Workshop Topics: data analysis techniques, data selection, background models, timing and spectroscopy.
5. 03/08/2020 – 05/08/2020 – Online
AtomDB Workshop and Advanced Spectroscopy School Topics: Spectroscopy and spectral analysis of spectra in the X-band.
6. 19/06/2023 – 23/06/2023 – PALAZZO D'AVALOS, VASTO, ITALY
THE FIRST VASTO ACCRETION MEETING



7. 02/10/2023 – 02/10/2023 – Monte Porzio Catone, Rome, Italy
12th Young Researcher Meeting 2023

- Talks:

1. **Talk:** “A thick forest of emission lines in the soft x-ray spectrum of LMXB Scorpius X-1” at **Congresso Nazionale Oggetti Compatti XII** - 27/09/2022 – 30/09/2022 – Cefalù (Palermo)
2. **Talk:** “Swift J1357.2-0933: the high inclination black hole X-ray transient” at **THE FIRST VASTO ACCRETION MEETING** - 19/06/2023 – 23/06/2023 – PALAZZO D'AVALOS, VASTO, ITALY
3. **Talk:** “J1357.2-0933: the high inclination black hole X-ray transient” at **12th Young Researcher Meeting 2023** - 02/10/2023 – 02/10/2023 – Monte Porzio Catone, Rome, Italy

- Posters:

4. **“Spectral analysis of the low-mass X-ray pulsar 4U 1822-371: Reflection component in a high-inclination system”** at **The 9th Microquasar Workshop: Celebrating over 50 years of discovery** - 20/09/2021 – 24/09/2021 – Cagliari, Italia

Papers published:

PRIMO AUTORE:

1. **Anitra**, C. Miceli, T. Di Salvo, R. Iaria, N. Degenaar, M. Jon Miller, F. Barra, W. Leone, L. Burderi, “An X-ray view of emission lines in optical spectra: spectral analysis of the two LMXB systems Swift J1357.2-0933 and MAXI J1305-704.”-2023; Submitted to A&A.
2. **A. Anitra**, C. Miceli, T. Di Salvo, R. Iaria, L. Burderi, F. Barra, W. Leone; “H β spectroscopy of the high-inclination black hole transient Swift J1357.2-0933 during quiescence” – 2023- DOI: [10.1051/0004-6361/202346909](https://doi.org/10.1051/0004-6361/202346909).
3. **A. Anitra**, T. Di Salvo, R. Iaria, L. Burderi, A.F. Gambino, S.M. Mazzola, A. Marino, A. Sanna, A. Riggio, “Spectral analysis of the low-mass X-ray pulsar 4U 1822-371: Reflection component in a high inclination system.” - 2021 2021, AA, 654, id. A160.

CO-AUTORE:

4. “The accretion/ejection link in the neutron star X-ray binary 4U 1820-30 I: a boundary layer-jet coupling?”- 2023- A. Marino, T. D. Russell, M. Del Santo, A. Beri, A. Sanna, F. Coti Zelati, N. Degenaar, D. Altamirano, E. Ambrosi, **A. Anitra**, F. Carotenuto, A. D’Ai, T. Di Salvo, A. Manca, S. E. Motta, C. Pinto, F. Pintore, N. Rea, J. Van den Eijnden.
5. “First Detection of X-Ray Polarization from the Accreting Neutron Star 4U 1820-303” - 2023 - Alessandro Di Marco, Fabio La Monaca, Juri Poutanen, Thomas D. Russell, **Alessio Anitra** et al.



6. Discovery of a variable energy-dependent X-ray polarization in the accreting neutron star GX 5-1 – 2023 - Sergio Fabiani , Fiamma Capitanio , Rosario Iaria , Juri Poutanen, Andrea Gnarini, Francesco Ursini , Ruben Farinelli , Anna Bobrikova, James F. Steiner , Jiri Svoboda , **Alessio Anitra** et al.
7. “Fe K and Fe K line detection in the NuSTAR spectrum of the ultra-bright Z source Scorpius X-1.” - 2021 -S. M. Mazzola, R. Iaria, T. Di Salvo, A. Sanna, A. F. Gambino, A. Marino, E. Bozzo, C. Ferrigno, A. Riggio, **A. Anitra** and L. Burderi, 2021, AA, 654, id. A102.
8. “Grail Quest HERMES: Hunting for gravitational wave electromagnetic counterparts and probing space-time quantum foam.” – 2020 - L. Burderi, T. Di Salvo, A. Riggio, A. F. Gambino, A. Sanna, F. Fiore, F. Amarilli, L. Amati, F. Ambrosino, G. Amelino-Camelia, **A. Anitra** et al., Proceedings of SPIE - The International Society for Optical Engineering, 2020, 11444, 114444Y.
9. “Spectral analysis of the “faint” AMXP Swift J1749.4-2807 during its 2021 outburst.” - 2022 - A. Marino, **A. Anitra**, S. Mazzola, A. Sanna, T. Di Salvo, A. Riggio, R. Iaria, L. Burderi.
10. “Spectral analysis of the AMXP during its 2018 outburst.” – 2022 - A. Manca, A.F. Gambino, A. Sanna, G. K. Jaisawal, T. Di Salvo, R. Iaria, S. M. Mazzola, A Marino, **A Anitra**, E Bozzo, A Riggio, L Burderi.
11. “On the peculiar long-term orbital evolution of the eclipsing accreting millisecond X-ray pulsar SWIFT J1749.4 – 2807” – 2022 - A. Sanna, L. Burderi, T. Di Salvo, A. Riggio, D. Altamirano, A. Marino, P. Bult, T. E. Strohmayer, S. Guillot, C. Malacaria, M. Ng, G. Mancuso, S. M. Mazzola, A. C. Albayati, R. Iaria, A. Manca, N. Deiosso, C. Cabras, **A. Anitra**.
12. “Quantum gravity with THESEUS” - 2021 -Burderi, L. ; Sanna, A. ; Di Salvo, T. ; Riggio, A. ; Iaria, R. ; Gambino, A. F. ; Manca, A. ; **Anitra, A.** ; Mazzola, S. M. ; Marino, A.
13. “Timing techniques applied to distributed modular high-energy astronomy: the H.E.R.M.E.S. project” – 2020 - Sanna, Andrea ; Burderi, Luciano ; Di Salvo, Tiziana ; Fiore, Fabrizio ; Riggio, Alessandro ; Gambino, Angelo ; Lavagna, Michèle ; Bertacin, Roberto ; Evangelista, Yuri ; Campana, Riccardo ; Fuschino, Fabio ; Lunghi, Paolo ; Monge, Ángel ; Negri, Barbara ; Pirrotta, Simone ; Puccetti, Simonetta ; Amarilli, Fabrizio ; Ambrosino, Filippo ; Amelino-Camelia, Giovanni ; **Anitra, Alessio** et al.



14. “The scientific payload on-board the HERMES-TP and HERMES-SP CubeSat missions” - 2020 - Y. Evangelista, F. Fiore, F. Fuschino, R. Campana, F. Ceraudo, E. Demenev, A. Guzman, C. Labanti, G. La Rosa, M. Fiorini, M. Gandola, M. Grassi, F. Mele, G. Morgante, P. Nogara, R. Piazzolla, S. Pliego Caballero, I. Rashevskaya, F. Russo, G. Sciarrone, G. Sottile, D. Milankovich, A. Pál, F. Ambrosino, N. Auricchio, M. Barbera, P. Bellutti, G. Bertuccio, G. Borghi, J. Cao, T. Chen, G. Dilillo, M. Feroci, F. Ficorella, U. Lo Cicero, P. Malcovati, A. Morbidini, G. Pauletta, A. Picciotto, A. Rachevski, A. Santangelo, C. Tenzer, A. Vacchi, L. Wang, Y. Xu, G. Zampa, N. Zampa, N. Zorzi, L. Burderi, M. Lavagna, R. Bertacin, P. Lunghi, A. Monge, B. Negri, S. Pirrotta, S. Puccetti, A. Sanna, F. Amarilli, G. Amelino-Camelia, M. Bechini, M. Citossi, A. Colagrossi, S. Curzel, G. Della Casa, M. Cinelli, M. Del Santo, T. Di Salvo, C. Feruglio, F. Ferrandi, M. Fiorito, D. Gacnik, G. Galgóczi, A. F. Gambino, G. Ghirlanda, A. Gomboc, M. Karlica, P. Efremov, U. Kostic, A. Clerici, B. Lopez Fernandez, A. Maselli, L. Nava, M. Ohno, D. Ottolina, A. Pasquale, M. Perri, M. Piccinin, J. Prinetto, A. Riggio, J. Ripa, A. Papitto, S. Piranomonte, F. Scala, D. Selcan, S. Silvestrini, T. Rotovnik, E. Virgilli, I. Troisi, N. Werner, G. Zanotti, **A. Anitra**, A. Manca, A. Clerici
15. “The HERMES-technologic and scientific pathfinder” – 2020 - F. Fiore, L. Burderi, M. Lavagna, R. Bertacin, Y. Evangelista, R. Campana, F. Fuschino, P. Lunghi, A. Monge, B. Negri, S. Pirrotta, S. Puccetti, A. Sanna, F. Amarilli, F. Ambrosino, G. Amelino-Camelia, **A. Anitra**, N. Auricchio, M. Barbera, M. Bechini, P. Bellutti, G. Bertuccio, J. Cao, F. Ceraudo, T. Chen, M. Cinelli, M. Citossi, A. Clerici, A. Colagrossi, S. Curzel, G. Della Casa, E. Demenev, M. Del Santo, G. Dilillo, T. Di Salvo, P. Efremov, M. Feroci, C. Feruglio, F. Ferrandi, M. Fiorini, M. Fiorito, F. Frontera, D. Gacnik, G. Galgoczi, N. Gao, A. F. Gambino, M. Gandola, G. Ghirlanda, A. Gomboc, M. Grassi, A. Guzman, M. Karlica, U. Kostic, C. Labanti, G. La Rosa, U. Lo Cicero, B. Lopez-Fernandez, P. Malcovati, A. Maselli, A. Manca, F. Mele, D. Milankovich, G. Morgante, L. Nava, P. Nogara, M. Ohno, D. Ottolina, A. Pasquale, A. Pal, M. Perri, R. Piazzolla, M. Piccinin, S. Pliego- Caballero, J. Prinetto, G. Pucacco, A. Rashevsky, I. Rashevskaya, A. Riggio, J. Ripa, F. Russo, A. Papitto, S. Piranomonte, A. Santangelo, F. Scala, G. Sciarrone, D. Selcan, S. Silvestrini, G. Sottile, T. Rotovnik, C. Tenzer, I. Troisi, A. Vacchi, E. Virgilli, N. Werner, L. Wang, Y. Xu, G. Zampa, N. Zampa, G. Zanotti
16. “Confirmation of the presence of a CRSF in the NICER spectrum of X 1822-371” – 2023 - R. Iaria, T. Di Salvo, **A. Anitra**, F. Barra, L. Burderi, A. Sanna, A. Riggio Submitted to A&A 2023
17. “Soft-state optical spectroscopy of the black hole MAXI J1305-704” – 2023 - C. Miceli, D. Mata Sánchez, **A. Anitra**, T. Muñoz-Darias, T. Di Salvo, R. Iaria, A. Marino, M. Del Santo, M. Armas-Padilla, N. Degenaar, J.M. Miller, M. Reynolds Submitted to A&A 2023



Thesis title:

Accretion Disc Tomography in Low-Mass X-Ray Binaries: A Multi wavelength approach

Abstract:

X-ray binaries, composed of a compact object accreting matter from a companion star, serve as ideal astrophysical laboratories for examining phenomena such as General Relativity. Particularly, the study of accretion discs in low-mass X-ray binary systems not only offers pivotal clues to the physics of accretion but also can unravel the geometry of these systems. The heart of this thesis is a multi-wavelength temporal and spectral analysis of these systems, extending from optical to X-ray wavelengths.

My first work delves into the spectral analysis of the low-mass X-ray pulsar 4U 1822-371. This study reveals for the first-time significant evidence of a reflection component in the x-ray spectrum of a high inclination source and provides updated orbital ephemerides. The analysis contributes to understanding the system's geometry proposing a unique configuration for the source.

With my second project I broadened the scope of my analysis to the optical range, analysing double-peaked H β line profile in the optical spectrum of Swift J1357.2-0933, a transient LMXB hosting one of the galaxy's most massive stellar-mass black hole candidates. This investigation not only estimated the black hole's systemic and radial velocity but also uncovered compelling evidence of a narrow core within the H β emission profile.

This work led me to develop a novel approach, applying X-ray spectral models to optical data. In my last work, I have introduced a method to model the optical H α and H β line profiles using a non-relativistic version of the diskline model. I applied the method to two sample sources, Swift J1357.2-0933 and MAXI J1305-704, providing estimates of the inner and outer radius of the emitting region of the disc and even of an inclination angle that matches perfectly the one reported in literature, but with higher precision.

This comprehensive approach offers new insights into the geometry of LMXBs, constraining critical parameters such as the inclination angle of the accretion disk, its size, and the temperature and ionization states across different disk regions. These parameters are not only fundamental to understanding the nature of the accretion process but can also provide a topographic map of the disc, shading light on whole structure of the disc and the physics that govern it.

The PhD Board Dean

Prof. Marco Cannas



Allegato 3

PHD IN PHYSICAL AND CHEMICAL SCIENCES, XXXVI COURSE

PhD Candidate: ...Yerong Xu...

Transcript of Records

Tutor: Dr. Giancarlo Cusumano

Cotutor: Dr. Ciro Pinto

Courses/school/exam scores:

- Exam for “End-to-end simulations with SIXTE” workshop, 30/10/2023
- Exam for course “Millisecond Pulsars: Theory and Observations”, lecturer: Prof. T. D. Salvo, 07/12/2021-13/01/2022
- Exam for “Chandra Data Science” Summer School, 25/01/2021

Research and training periods abroad

- Erasmus+ Extra EU study program, Massachusetts Institute of Technology, 02/01/2023-11/06/2023
- European Space Agency Archival Research Visitor program, European Space Astronomy Centre, 10/09/2022-04/12/2022

Papers published:

- **Y. Xu**, C. Pinto, D. Rogantini, et al., *Constraints on the ultrafast outflows in the narrow-line Seyfert 1 galaxy Mrk 1044 from high-resolution time-and flux-resolved spectroscopy*, Monthly Notices of the Royal Astronomical Society, 2023
- **Y. Xu**, C. Pinto, E. Kara, et al., *Ejection-accretion connection in NLS1 AGN 1H 1934-063*, Monthly Notices of the Royal Astronomical Society, 2022
- **Y. Xu**, C. Pinto, S. Bianchi, et al., *Wind-luminosity evolution in NLS1 AGN 1H 0707-495*, Monthly Notices of the Royal Astronomical Society, 2021
- **Y. Xu**, J. A. Garcia, D. J. Walton, et al., *The Nature of Soft Excess in ESO 362-G18 Revealed by XMM-Newton and NuSTAR Spectroscopy*, The Astrophysical Journal, 2021
- B. P. Thomas, J. C. Wheeler, V. V. Dwarkadas, et al., *Seven Years of SN 2014C: A Multiwavelength Synthesis of an Extraordinary Supernova*, The Astrophysical Journal, 2022
- M. L. Parker, W. N. Alston, L. Harer, et al., *The nature of the extreme X-ray variability in the NLS1 1H 0707-495*, Monthly Notices of the Royal Astronomical Society, 2021



Conferences/workshop attended:

- Talks:

- *Ultra-fast outflow responses in highly accreting supermassive black holes*, on the conference “Young Astronomers on Galactic Nuclei 2023” hosted by INAF-IASF Palermo, on 20/10/2023
- *Ultra-fast outflow responses in highly accreting supermassive black holes*, on the conference “Chandra High Resolution X-ray Spectroscopy workshop” hosted by Chandra Team, on 02/08/2023
- *Ultra-fast outflow responses in highly accreting supermassive black holes*, on the conference “X-ray Universe 2023” hosted by European Space Astronomy Centre, on 14/06/2023
- *Ultra-fast Outflows around highly-accreting supermassive black holes*, on the High Energy Astrophysics Seminar, Harvard–Smithsonian Center for Astrophysics, on 24/03/2023
- *Ultra-fast Outflows around highly-accreting supermassive black holes*, on the Chandra HETG group meeting, Massachusetts Institute of Technology, on 09/03/2023
- *Ultra-fast Outflows around highly-accreting supermassive black holes*, on the Erin Kara’s group meeting, Massachusetts Institute of Technology, on 03/03/2023
- *Ejecta-accretion connection in highly-accreting supermassive black holes*, on the Conference “Black hole accretion under the X-ray microscope” hosted by European Space Astronomy Centre, on 14-17/06/2022
- *Ejecta-accretion connection in highly-accreting supermassive black holes*, on the Conference “Latest advances in X-ray spectroscopy and polarimetry” hosted by University of Roma Tor Vergata, on 18-20/05/2022
- *What Drives the Wind-luminosity Evolution in NLS1 1H 0707-495?*, on the Conference “50 years astronomical X-ray spectroscopy in the Netherlands” hosted by SRON, on 17-19/01/2022
- *Wind-luminosity evolution 1H0707-495*, on the Cosimo Bambi’s group meeting, Fudan University, on 26/10/2021
- *What Drives the Wind-luminosity Evolution in NLS1 1H 0707-495?*, on the Conference “Black hole accretion disc winds” hosted by University of Durham, on 06-09/09/2021
- Eight presentations on the weekly Journal Club (21/12/2020, 17/06/2021, 06/04/2022 and 29/11/2022) and internal seminars (04/11/2020, 01/06/2022, 21/03/2023 and 21/11/2023) at INAF-IASF Palermo

- Posters:

- *Ultra-fast Outflows in highly-accreting supermassive black holes*, on the Conference “Exploring the Hot and Energetic Universe: the third scientific conference dedicated to the Athena X-ray Observatory” hosted by ATHENA team, on 07-10/11/2022



- Attended:

- Summer school “Life and death: From stars to compact objects”, hosted by University of Padova, 28/08-03/09/2022
- Workshop “Chandra Data Science: Novel Methods in Computing and Statistics for X-ray Astronomy”, hosted by Chandra team, 17-19/08/2021, 24-26/08/2021, 30/08/2021-01/09/2021
- Workshop “The high-resolution X-ray and UV spectroscopy capability building workshop”, hosted by Nanjing University, 15-18/08/2022
- Workshop “End-to-end simulations with SIXTE: An online workshop 2022”, hosted by ATHENA team, 29-31/03/2022
- Workshop “CSST-Euclid-Roman Workshop”, hosted by Leiden Observatory, 21-25/06/2021

Thesis title: A high-resolution study of powerful winds in highly accreting supermassive black holes

Abstract:

An active galactic nucleus (AGN) is powered by the accretion of matter infalling onto a supermassive black hole (SMBH), found at the core of most galaxies. The accretion process releases an enormous amount of radiation, while concurrently propelling matter away through winds, especially for those accreting approach or exceed the Eddington limit. Black holes at Eddington accretion rates are growing fast but are also expected to launch powerful winds of hot plasmas due to the extreme radiation pressure from the underlying accretion disk. These outflows, when intersecting our line of sight to the radiation source, leave imprints in X-ray spectra of the accretion disk in the form of Doppler-shifted lines. AGN winds play a critical role in regulating SMBH growth and the host galaxy’s evolution by carrying away a significant portion of infalling matter. Notably, certain AGN outflows, known as ultra-fast outflows (UFOs), can achieve speeds exceeding 3% and even reach 30% of the speed of light. Due to their extreme velocities, UFOs are regarded as a promising candidate to affect the galaxy evolution by depositing significant kinetic energy into the surrounding gas, thereby heating the interstellar medium and quenching the star formation rate of the host galaxy. However, the uncertainties in the geometries, launching mechanisms and outflow rates of such outflows imply a substantial uncertainty in determining their effects on SMBH evolution and the impacts on host galaxies.

By using both the currently most advanced photoionization modelling method and the data from the by far best instrument for soft X-ray high-resolution spectroscopy, XMM-Newton Reflection Grating Spectrometer (RGS), I studied the nature of UFOs in soft X-ray bands of a super-Eddington narrow-line Seyfert 1 (NLS1) galaxy and a high-Eddington NLS1 AGN and extend the analysis to a large sample of high-Eddington AGN. UFOs in the soft X-ray bands are largely overlooked before my works and commonly exhibit a cool temperature. My results reveal that UFOs in these systems are driven by the radiation pressure and are sufficiently energetic to affect the evolution of their host galaxies, while the radiative acceleration may decrease as the accretion rate increases, probably due to the change in the geometry of accretion flows. Additionally, I also achieved the first discovery of evidence for the connection between the accretion inflows and UFOs in the soft X-ray band of an NLS1 galaxy.

The PhD Board Dean

Prof. Marco Cannas