POLITECNICO MILANO 1863

PUBLIC SELECTION ESTABLISHED WITH DIRECTOR'S DECREE NO. 2022_PRO_DCMC_1 OF 03/02/2022 PURSUANT TO THE NOTICE PUBLISHED IN THE OFFICIAL GAZETTE NO. 01/03/2022, n. 17 FOR 1 POSITION AS FULL PROFESSOR FOR THE COMPETITION SECTOR 03/B2 - PRINCIPLES OF CHEMISTRY FOR APPLIED TECHNOLOGIES - SDS CHIM/07 - PRINCIPLES OF CHEMISTRY FOR APPLIED TECHNOLOGIES, PURSUANT TO ART. 18 - LAW 240/2010, AT THE POLITECNICO DI MILANO - DEPARTMENT OF CHEMISTRY, MATERIALS AND CHEMICAL ENGINEERING "GIULIO NATTA" (PROCEDURE CODE 2022_PRO_DCMC_1).

FINAL REPORT

The Selection Board, appointed with RD Index No. 3307 ref. No. 90831 of 01 April 2022, composed by the following Professors:

Prof. RAOS Guido - Politecnico di Milano;
Prof. PASSERINI Stefano - Karlsruher Institut für Technologie;
Prof. STINGELIN Natalie - Georgia Institute of Technology,

met on 4th May 2022 at 16:00 CEST, for the first teleconference meeting.
Each board member was connected from his/her workstation.

At the start of the session the members of the Selection Board named the Chairman and the Secretary of the Selection Board:

STEFANO PASSERINI, FULL PROFESSOR at the KARLSRUHER INSTITUT FÜR TECHNOLOGIE, Chairman;
GUIDO RAOS, FULL PROFESSOR at the POLITECNICO DI MILANO, Secretary.

Each member of the board declared not to have conjugal nor family relationship or other degree of kinship or affinity up to the fourth degree, not to be in same-sex civil union (as per art. 1 of Law No. 76 of 20.05.2016) and not to form a cohabiting couple (as per art. 1, paragraphs 37 et seq. of Law No. 76 of 20.05.2016) with the other members of this board and that there were no reasons for abstention pursuant to arts. 51 and 52 of the Civil Procedure Code.

The members of the Selection Board and the Secretary declared, pursuant to art. 35-bis of Legislative Decree 165/2001, not to have criminal convictions, even with non-definitive sentences, for offences provided for in Chapter I, Title II of the second book of the Criminal Code.

The Selection Board established the criteria and the parameters according to which the assessment was carried out, and set the minimum score below which the candidate shall not be included in the ranking of candidates.

On 26th May 2022 at 16:00 CEST, the Selection Board met in teleconference to inspect the list of applicants, who were:

1) FAMULARI, Antonino
2) MACCHI, Piero

Each member of the board declared not to have conjugal nor family relationship or other degree of kinship or affinity up to the fourth degree, not to be in same-sex civil union (as per art. 1 of Law No. 76 of 20.05.2016) and not to form a cohabiting couple (as per art. 1, paragraphs 37 et seq. of Law No. 76 of 20.05.2016) with the candidates and stated that there were no reasons for abstention pursuant to arts. 51 and 52 of the Civil Procedure Code.

Pursuant to the examination and after adequate evaluation, the Selection Board assigned a score to each of the established criteria and a judgment to each publication submitted by the candidate; furthermore, the board evaluated the knowledge of the English language.

Therefore the board, considering the sum of the scores given, expressed a collective judgment in relation to the quantity and the quality of publications, evaluating the overall productivity of the applicant, also with regard to his/her period of activity.

The above-mentioned judgments are attached to this report and they are an integral part of it (Attachment No. 1 to this final report).

The Selection Board drew up, according to the majority of its members, a ranking of candidates selected to carry out the scientific/teaching functions for which the selection was called, in a number equal to a maximum of five times the number of positions available in the competition (Attachment No. 2 to this final report).

THE SELECTION BOARD

Prof. Stefano Passerini (Chairman) _____

Prof. Natalie Stingelin (Member) _____

Prof. Guido Raos (Secretary) _____

Firmato digitalmente da:GUIDO RAOS
Organizzazione:
POLITECNICO DI
MILANO/80057930150

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ATTACHMENT No. 1 to the FINAL REPORT

CRITERIA	Quality of scientific and/or project production, assessed on the basis of criteria and parameters recognized by the international scientific community of reference	Teaching activity at the university level in Italy or abroad	Scientific responsibility for funded research projects	Results obtained in technology transfer in terms of participation in the creation of new enterprises (spin off), development, use and marketing of patents	Total
FAMULARI Antonino	30	20	20	2	72
MACCHI Piero	37	20	25	0	82

CANDIDATE: FAMULARI Antonino

CURRICULUM:
Born in 1969, male, Italian nationality. MSc in chemistry at the Università degli Studi di Milano (UNIMI), with a 110/110 mark (1994). PhD in chemical science at UNIMI, with a thesis on the development of theoretical methods for intermolecular forces (1997). He spent about three years as a post-doctoral researcher at UNIMI and at the CNR-ISTM center, also in Milano (1998-2000). He was a full-time researcher at the same CNR center for a few months in 2001. He has been at the Politecnico di Milano (POLIMI) since 2001, first as an assistant professor of chemistry, and then as an associate professor (from 2014 onward). He obtained the national habilitation for the position of full professor in the 03/B2 area, first in 2014 and then again in 2018.

SUBMITTED PUBLICATIONS:

No.	**Title**	**Judgment**
1	Kinetically Controlled Fast Crystallization of M12L8 Poly-[n]-catenanes Using the 2,4,6-Tris(4-pyridyl)benzene Ligand and ZnCl2 in an Aromatic Environment	Excellent
2	New basis set superposition error free ab initio MOVB interaction potential: Molecular-dynamics simulation of water at critical and supercritical conditions	Excellent
3	2,3-exo-Disyndiotactic Polynorbornene: a Crystalline Polymer with Tubular Helical Molecular Structure	Good
4	A Solid State Density Functional Study of Crystalline Thiophene-Based Oligomers and Polymers	Very good
5	Intramolecular CH/π interactions in alkylaromatics: Monomer conformations for poly(3-alkylthiophene) atomistic models	Very good
6	Synthesis of Chelating Complexes through Solid-State Dehydrochlorination Reactions via Second-Sphere-Coordination Interaction with Metal Chlorides: A Combined Experimental-Molecular Modeling Study	Good
7	On the inter-ring torsion potential of regioregular P3HT: a first principles reexamination with explicit side chains	Good
8	Structure–Photoluminescence Correlation for Two Crystalline Polymorphs of a Thiophene–Phenylene Co-Oligomer with Bulky Terminal Substituents	Very good

9	First detailed determination of the Molecular Conformation and the Crystalline Packing of a Chiral Poly(3-alkylthiophene): Poly-3-(S)-2-methylbutylthiophene	Very good
10	Ordered Stacking of Regioregular Head-to-Tail Polyalkylthiophenes: Insights from the Crystal Structure of Form I' Poly(3-n-butylthiophene)	Very good
11	Nucleophilicity and electrophilicity of the C(sp(3))-H bond: methane and ethane binary complexes with iodine	Good
12	Insights into the electron-donating and withdrawing effect of the functional groups on mechanochemical dehydrochlorination reactions	Very good
13	Gas-Solid Chemisorption/Adsorption and Mechanochemical Selectivity in Dynamic Nonporous Hybrid Metal Organic Materials	Excellent
14	N-Alkyl substituted 1 H-benzimidazoles as improved n-type dopants for a naphthalene-diimide based copolymer	Very good
15	Dual-Mode Light Transduction through a Plastically Bendable Organic Crystal as an Optical Waveguide	Excellent

Overall collective judgement

QUALITY OF SCIENTIFIC AND/OR PROJECT PRODUCTION, ASSESSED ON THE BASIS OF CRITERIA AND PARAMETERS RECOGNIZED BY THE INTERNATIONAL SCIENTIFIC COMMUNITY OF REFERENCE:
The candidate has published about 102 articles in journals indexed in the ISI WOS database, that all together have collected nearly 2300 citations, with an H-index=29.
His expertise and research interests are described by the following keywords: material characterization, molecular modelling, structure-activity relationship, X-Ray diffraction: WAXS and SAXS techniques, quantum chemistry, electronic density, electronic structure. The methods and code for intermolecular interactions that he developed in his PhD and postdoc periods are part of GAMESS-US, a widely used molecular electronic structure program.
The candidate has submitted 15 publications, in the areas of materials and computational chemistry. Among these, he is first author in two manuscripts and corresponding author in four.

DIDACTIC ACTIVITIES CARRIED OUT IN ITALIAN OR FOREIGN UNIVERSITIES OR BODIES:
Since 2002, he has the responsibility of general chemistry courses for BSc engineering students at POLIMI. In 2000-2004, he was a teaching assistant in other general chemistry courses at POLIMI. In 2005-2007, he taught also an “environmental chemistry” course at POLIMI. Since 2017, he has had the responsibility of a “chemistry of materials” course, at the MSc level (in English). He has also taught within different editions of a PhD course on “Structural and statistical properties of polymers” (2005-2016) and a PhD course on “Simulation of molecular systems for chemistry, materials and biology” (2005-present). In 2017, he was in charge of the organization of one edition of the latter. He declares the supervision of about 20 PhD and master students. He is a co-author of a chemistry exercise textbook (4 editions).

SCIENTIFIC RESPONSIBILITY FOR FUNDED RESEARCH PROJECTS:
Principal investigator within a PRIN 2004 project on “Nano-analytical systems for chem & bio-sensing” (91500 Euros, 2005-2007), a PRIN 2006 project on “Organic functional materials: characterization of self assembly processes and advanced applications” (60715 Euros, 2007-2009), a FARB 2011 project funded by POLIMI on “Molecular modeling of CO2 absorption in ionic liquids” (unspecified amount, 2011-2013). Principal investigators in four projects for the allocation of supercomputer time by CILEA and CINECA (2011, 2013, 2014, 2016). Participant in ten other competitively funded research projects (FIRB or PRIN by MIUR, Fondazione CARIPLO, PRISMA by INSTM, one FP7 project by the EU).

RESULTS OBTAINED IN TECHNOLOGY TRANSFER IN TERMS OF PARTICIPATION IN THE CREATION OF NEW ENTERPRISES (SPIN OFF), DEVELOPMENT, USE AND MARKETING OF PATENTS:
Declares three patents in his CV. The attachments include an Italian and an international patent application on stereoregular polymers and copolymers of norbornene, filed in 2008 and 2010, respectively.

SCRUTINY OF THE DEGREE OF KNOWLEDGE OF THE ENGLISH LANGUAGE:
Very good knowledge of the English language, demonstrated by the publications for which he is a corresponding author, participation at international meetings, and teaching activity in English at POLIMI.

CANDIDATE: MACCHI Piero

CURRICULUM:
Born in 1970, male, Italian nationality. MSc in chemistry at the Università degli Studi di Milano (UNIMI), with a mark of 110/110 *cum laude* (1994). PhD in chemical science at UNIMI, with a thesis in the area of chemical crystallography and bonding in metal carbonyls (1997). He has been a research technician at UNIMI (1998-1999 and 2000-2001), assistant professor at the University of Aarhus (1999-2000), assistant professor again at UNIMI (2002-2008), research group leader and later associate professor at the University of Bern (2009-2019), associate professor at the Politecnico di Milano (POLIMI, 2019-present). Invited professor at the University of Bratislava (2008) and of Lorraine (2016). Several research stays at the State University of New York at Buffalo (2000, 2003, 2004, 2006). Currently holds the national habilitation to full professor in two chemical areas (03/B2 and 03/A2). He was elected to institutional roles at UNIMI, Bern and POLIMI. He has had institutional roles in the Italian and the Swiss crystallographic associations, most notably president of the latter (2015-2018). Currently affiliated also to the Italian Institute of Technology (CNST@polimi). The candidate has a notable international experience and visibility.

SUBMITTED PUBLICATIONS:

No.	Title	Judgment
1	Experimental electron density studies for investigating the metal π-ligand bond: the case of bis(1,5-cyclooctadiene) nickel	Excellent
2	The connubium between crystallography and quantum mechanics	Excellent
3	Electron Density and Dielectric Properties of highly porous MOFs: binding and mobility of guest molecules in Cu3(BTC)2 and Zn3(BTC)2	Excellent
4	Pressure-Induced Polymerization and Electrical Conductivity of a Polyiodide	Excellent
5	Putting pressure on aromaticity along with in situ experimental electron density of a molecular crystal	Excellent
6	Experimental and Theoretical Electron Density Analysis of Copper Pyrazine Nitrate Quasi-Low-Dimensional Quantum Magnets	Excellent
7	Solid-State Reversible Nucleophilic Addition in a Highly Flexible MOF	Excellent
8	Resonant structures and electron density analysis	Good
9	Polyfunctional Inorganic-Organic Hybrid Materials: An Unusual Kind of NLO Active Layered Mixed Metal Oxalates with Tunable Magnetic Properties and Very Large Second Harmonic Generation	Excellent
10	The Electron Density of Bridging Hydrides Observed via Experimental and Theoretical Investigations on [Cr2(μ2-H)(Co)10]-	Good
11	Chemical bonding in transition metal carbonyl clusters: complementary analysis of theoretical and experimental electron densities	Excellent
12	Electron Density of Semi-Bridging Carbonyls. Metamorphosis of CO Ligands Observed via Experimental and Theoretical Investigations on [FeCo(CO)8]-	Excellent
13	Interanionic O−H···O Interactions: The Charge Density Point of View	Excellent
14	Charge density in transition metal clusters: supported vs. unsupported metal-metal interactions	Excellent
15	Experimental Electron Density in a Transition Metal Dimer: Metal−Metal and Metal−Ligand Bonds	Very good

Overall collective judgement

QUALITY OF SCIENTIFIC AND/OR PROJECT PRODUCTION, ASSESSED ON THE BASIS OF CRITERIA AND PARAMETERS RECOGNIZED BY THE INTERNATIONAL SCIENTIFIC COMMUNITY OF REFERENCE:

The candidate has published about 149 articles in journals indexed in the ISI WOS database, that all together have collected nearly 4900 citations, with an H-index=35. Editor and co-author of one contributed book, one monography and one textbook, on the topics of charge density analysis and quantum crystallography. Co-editor of Acta Crystallographica Sect. B (IUCr/Wiley) and of Crystals (MDPI). Young Investigator award by the Italian Crystallographic Association (2002). Vice-chair and then chair of a Gordon Research Conference on "Electron distribution and chemical bonding" (2010 and 2013). Organizer or member of the scientific committee of several other national (Italian or Swiss) and international conferences, including the CECAM workshop "Second discussion meeting on quantum crystallography" (held online in 2021).

The candidate's core scientific activity can be classified under the labels of "quantum crystallography" and "high-pressure chemistry". The first one started during in PhD (1996) with the analysis of detailed electron densities of metal carbonyls, and continues to this day on other materials, such as organic crystals and organometallic polymers. He is a (co)author of the software XD, for the analysis of experimental electron densities, and of Polarber, for the prediction of dielectric properties of crystals. Research activity on high-pressure chemistry started at Bern in the mid-2000's. This research has produced significant results in areas such as pressure-induced polymerization, magnetism and chemical reactions in metal-organic framework. He has a long-term cooperation project with the PSI (Villigen, CH), to develop the instrumentation for diffraction experiments under high pressure and in electric fields.

The candidate has submitted 15 publications, in the areas of structure and electronic properties of mainly inorganic and metal-organic materials. Among these, he is first author in nine manuscripts and corresponding author in fourteen.

DIDACTIC ACTIVITIES CARRIED OUT IN ITALIAN OR FOREIGN UNIVERSITIES OR BODIES:

At Aarhus, UNIMI, Bern and POLIMI he has taught several courses covering a broad range of topics, mainly related to general and inorganic chemistry, crystallography and quantum chemistry, from the BSc to the PhD level. At POLIMI, he has been the director and teacher of the PhD course "Synchroton X-ray diffraction, spectroscopy and imaging". Director/organizer of four international schools in the areas of crystallography and charge density analysis, most notably of the 52nd edition of the International School of Crystallography at Erice (2018).

Since 1999, he has been supervisor of more than 25 bachelor thesis projects (UNIMI, Bern, POLIMI), 9 master theses (UNIMI and Bern), 9 PhD theses (UNIMI, Bern and POLIMI), co-supervisor or external supervisor of 6 PhD thesis. At Bern, has been advisor to five post-doctoral researchers.

Member of the PhD board in Materials Engineering at POLIMI (2021-present).

SCIENTIFIC RESPONSIBILITY FOR FUNDED RESEARCH PROJECTS:
Very active in securing research funding during his period at the University of Bern (2009-2019), leading to about 2000000 CHF as single PI or principal PI in projects funded by Swiss agencies (SNF, CRUS), and partner in two projects funded by SNF and by the Paul Scherrer Institute, for another 500000 CHF. Co-proponent in the Swiss national competence center MARVEL. At Bern he obtained also more than 200000 CHF through consulting, analysis and third-party funds. During his early career in Italy (2001-2008), he participated in four PRIN or FIRB projects, funded by MIUR. After his return to Italy, he has been a participant in one project funded by Regione Lombardia (2020-2023).

RESULTS OBTAINED IN TECHNOLOGY TRANSFER IN TERMS OF PARTICIPATION IN THE CREATION OF NEW ENTERPRISES (SPIN OFF), DEVELOPMENT, USE AND MARKETING OF PATENTS:
The candidate reports no activity in this area.

SCRUTINY OF THE DEGREE OF KNOWLEDGE OF THE ENGLISH LANGUAGE:
Very good knowledge of the English language, demonstrated by the publications for which he is a corresponding author, teaching at foreign institutions, and by more than 70 presentations and seminars at conferences, schools and workshop (7 keynote and 3 plenary lectures).

THE SELECTION BOARD

Prof. Stefano Passerini (Chairman) _____

Prof. Natalie Stingelin (Member) _____

Prof. Guido Raos (Secretary) _____

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ATTACHMENT No. 2 to the FINAL REPORT

MERIT RANKING

SURNAME AND NAME	Overall score
MACCHI Piero	82
FAMULARI Antonino	72

Milan, 26th May 2022.

THE SELECTION BOARD

Prof. Stefano Passerini (Chairman) _____

Prof. Natalie Stingelin (Member) _____

Prof. Guido Raos (Secretary) _____