Antonino Famulari – Curriculum Vitae

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Antonino Famulari graduated in Chemistry with merit at the Università degli Studi di Milano in 1994 with the thesis: ”Parallel calculation in Quantum Monte Carlo” (Supervisors: Prof. G. Morosi and Dr P. Cremaschi). In 1998, he completed his PhD in the field of Molecular Modeling at the Università degli Studi di Milano. Title of the thesis: “Developement of ab inito theoretical methods for the study of intermolecular interactions” (Supervisor Prof. M. Raimondi, Coordinator Prof. C. Scolastico). During the PhD he spent more then 9 months working in foreign countries. In particular he visited the Department of Chemistry of the University of Liverpool (Prof. D.L. Cooper), the Department of Chemistry of the Iowa State University (Prof. M. S. Gordon) and the Department of Chemistry of the University of Copenaghen (Prof. S. Rettrup). He had a post doctoral research grant by the Consiglio Nazionale delle Ricerche (1998) and later a Contract of Research in the field of Chemical Science at the Dipartimento di Chimica Fisica ed Elettrochimica, Università degli Studi di Milano (1999-2001). In 2000 he was appointed at a Permanent Research position by the CNR center ISTM (Scienze e Tecnologie Molecolari) of Milan. In December 2001 he moved (role: Assistant Professor) to the Dipartimento di Chimica, Materiali e Ingegneria Chimica “Giulio Natta” of the Politecnico di Milano joining the research group of Prof. Allegra and Prof. Meille. Since 1 November 2014 he was appointed to an Associate Professor position. At the beginnings of his research activity, he worked on the development of new methods for the calculation of accurate intermolecular interactions; the approaches are available as standard options in general software such as GAMESS-US package. Currently he is working on: (i) Molecular Modeling of non-covalent interactions focusing to the study of molecules and macromolecules in the crystallization and self-organization processes (from molecular mechanics and dynamics to ab initio quantum mechanical approaches also including methods specific for solid phases) and (ii) X-ray scattering methodologies including both WAXD and SAXS techniques. Main research interests of the candidate are: a) structure and morphology of polymers, oligomers and molecules (in particular innovative materials in the field of the organic electronics, organic heterojunction photovoltaics and sensor and optical applications) and of polymer/clay composites and nano-composites aiming to the formulation of structure-property relationships; b) intermolecular interactions in ionic liquids and systems of biological interests. He collaborated with several international research groups (Professor M. S. Gordon, Iowa State University; Dr Carlo Gatti, CNR of Milan; Professor A.R. Khokhlov, Physics Department, Moscow State University; Professor D. L. Cooper, University of Liverpool;). He is the author of about 100 scientific papers on various international journals (1850 citations, H-index 24, SCOPUS, April 2018), 2 patents and more than 50 communications to international conferences. The values of the indexes used in national scientific qualifications are: 42 (normalized number of papers), 1005 (normalized citations) and 18 (normalized H-index). In 2014 he obtained 3 national scientific qualifications as Associate Professor (SSD: 03/B1 Principles of chemistry and inorganic systems, 03/B2 Chemical Foundations of Technologies and 03/C2 Industrial and applied chemistry) and 1 national scientific qualification as Full Professor (SSD: 03/B2). The last qualification (SSD: 03/B2) has been obtained also in 2018. Antonino Famulari was leader of projects in the field of PRIN financial support and of CINECA/LISA initiatives.

The teaching experience of the candidate was mainly in the basic courses of Chemistry for Engineering (bachelor Science) students with large classes (SSD:03/B2) but he is has also teaching activity in the framework of the Material Engineering (Master of Science) at Politecnico of Milan: "Structural Chemistry of Materials" (in English). He is co-author of a Chemistry exercises book (3 revised versions) for technical and scientific bachelor courses. In addition, the candidate has a teaching activity (in English) in the courses for PhD students at Politecnico di Milano: Molecular Modelling, Structure and statistical properties of polymers, Characterization techniques of materials (X ray diffraction WAXS and SAXS and thermal analysis). ORCID: 0000-0001-5287-1092

Recent relevant publications:

1)Li, H., Guo, F., Kou, M., Famulari, A., Fu, Q., Marti-Rujas, J. Gas-Solid Chemisorption/Adsorption and Mechanochemical Selectivity in Dynamic Nonporous Hybrid Metal Organic Materials (2017) Inorganic Chemistry, 56 (11), pp. 6584-6590. DOI: 10.1021/acs.inorgchem.7b00698

2) Baggioli, A., Meille, S.V., Famulari, A. Nucleophilicity and electrophilicity of the C(sp3)-H bond: Methane and ethane binary complexes with iodine (2017) Physical Chemistry Chemical Physics, 19 (36), pp. 24555-24565. DOI: 10.1039/c7cp03488a

3) Guo, F., Wang, Z., Zhang, J.-J., Famulari, A., Li, H.-T., Martí-Rujas, J. Insights into the electron-donating and withdrawing effect of the functional groups on mechanochemical dehydrochlorination reactions (2017) Dalton Transactions, 46 (29), pp. 9466-9471. DOI: 10.1039/c7dt01710c

4) Yu, H.-B., Li, H.-T., Zhang, P., Famulari, A., Guo, F., Bargigia, I., Martí-Rujas, J. Exploiting polymorphism in second sphere coordination: Thermal transformation, NLO properties and selective mechanochemical synthesis

(2016) CrystEngComm, 18 (14), pp. 2408-2412. DOI: 10.1039/c6ce00366d

5) Baggioli, A., Cavallotti, C.A., Famulari, A. Exploring short intramolecular interactions in alkylaromatic substrates (2016) Physical Chemistry Chemical Physics, 18 (42), pp. 29616-29628. DOI: 10.1039/c6cp03323g

6) Caronna, T., Mele, A., Famulari, A., Mendola, D., Fontana, F., Juza, M., Kamuf, M., Zawatzky, K., Trapp, O. A Combined Experimental and Theoretical Study on the Stereodynamics of Monoaza[5]helicenes: Solvent-Induced Increase of the Enantiomerization Barrier in 1-Aza-[5]helicene (2015) Chemistry - A European Journal, 21 (40), pp. 13919-13924. DOI: 10.1002/chem.201502288

7) Yu, H.-C., Li, L., Gao, J., Tong, J., Zheng, W., Cametti, M., Famulari, A., Meille, S.V., Guo, F., Martí-Rujas, J. Insights into the formation of chiral second sphere coordination complexes with aromatic tris amines: combined single crystal X-ray crystallography and molecular modeling analyses (2015) Dalton Transactions, 44 (36), pp. 15960-15965. DOI: 10.1039/c5dt02387d

8) Guo, F., Wang, X., Guan, H.-Y., Yu, H.-B., Li, L., Chen, S.-S., Famulari, A., Martí-Rujas, J. Tuning the inclusion properties and solid-state reactivity of second sphere adducts using conformationally flexible bidentate ligands (2015) Crystal Growth and Design, 15 (6), pp. 2842-2852. DOI: 10.1021/acs.cgd.5b00272

9) Liu, H.-L., Xie, Y.-F., Pan, Z.-G., Famulari, A., Guo, F., Zhou, Z., Martí-Rujas, J. Cyclic interconversion among molecular salts via neat grinding and related photoluminescence properties (2014) Crystal Growth and Design, 14 (12), pp. 6528-6536. DOI: 10.1021/cg5014329

10) Castiglione, F., Famulari, A., Raos, G., Meille, S.V., Mele, A., Appetecchi, G.B., Passerini, S. Pyrrolidinium-based ionic liquids doped with lithium salts: How does Li+ coordination affect its diffusivity? (2014) Journal of Physical Chemistry B, 118 (47), pp. 13679-13688. DOI: 10.1021/jp509387r

11) Sansotera, M., Gambarotti, C., Famulari, A., Baggioli, A., Soave, R., Venturini, F., Meille, S.V., Wlassics, I., Navarrini, W. Free-radical selective functionalization of 1,4-naphthoquinones by perfluorodiacyl peroxides (2014) Tetrahedron, 70 (34), pp. 5298-5309. DOI: 10.1016/j.tet.2014.05.024

12) Guan, H.-Y., Wang, Z., Famulari, A., Wang, X., Guo, F., Martí-Rujas, J. Synthesis of chelating complexes through solid-state dehydrochlorination reactions via second-sphere-coordination interaction with metal chlorides: A combined experimental-molecular modeling study (2014) Inorganic Chemistry, 53 (14), pp. 7438-7445. DOI: 10.1021/ic5007583

13) Nicolini, T., Famulari, A., Gatti, T., Martí-Rujas, J., Villafiorita-Monteleone, F., Canesi, E.V., Meinardi, F., Botta, C., Parisini, E., Meille, S.V., Bertarelli, C. Structure-photoluminescence correlation for two crystalline polymorphs of a thiophene-phenylene co-oligomer with bulky terminal substituents (2014) Journal of Physical Chemistry Letters, 5 (13), pp. 2171-2176. DOI: 10.1021/jz500925r

14) Baggioli, A., Famulari, A. On the inter-ring torsion potential of regioregular P3HT: A first principles reexamination with explicit side chains (2014) Physical Chemistry Chemical Physics, 16 (9), pp. 3983-3994. DOI: 10.1039/c3cp54688h

15) Guo, F., Shao, H.-D., Yang, Q., Famulari, A., Martí-Rujas, J. Mechanochemical dehydrochlorination and chelation reaction in the solid state: From a molecular salt to a coordination complex (2014) CrystEngComm, 16 (6), pp. 969-973. DOI: 10.1039/c3ce41900b

16) Galletta, M., Scaravaggi, S., Macerata, E., Famulari, A., Mele, A., Panzeri, W., Sansone, F., Casnati, A., Mariani, M. 2,9-Dicarbonyl-1,10-phenanthroline derivatives with an unprecedented Am(iii)/Eu(iii) selectivity under highly acidic conditions (2013) Dalton Transactions, 42 (48), pp. 16930-16938. DOI: 10.1039/c3dt52104d

17) Baggioli, A., Meille, S.V., Raos, G., Po, R., Brinkmann, M., Famulari, A. Intramolecular CH/π interactions in alkylaromatics: Monomer conformations for poly(3-alkylthiophene) atomistic models (2013) International Journal of Quantum Chemistry, 113 (18), pp. 2154-2162. DOI: 10.1002/qua.24472

18) Guo, F., Zhang, M.-Q., Famulari, A., Martí-Rujas, J. Solid state transformations in stoichiometric hydrogen bonded molecular salts: Ionic interconversion and dehydration processes3 (2013) CrystEngComm, 15 (31), pp. 6237-6243. DOI: 10.1039/c3ce40614h

19) Talaeemashhadi, S., Sansotera, M., Gambarotti, C., Famulari, A., Bianchi, C.L., Antonio Guarda, P., Navarrini, W. Functionalization of multi-walled carbon nanotubes with perfluoropolyether peroxide to produce superhydrophobic properties (2013) Carbon, 59, pp. 150-159. DOI: 10.1016/j.carbon.2013.03.003

20) Kozma, E., Kotowski, D., Catellani, M., Luzzati, S., Famulari, A., Bertini, F. Synthesis and characterization of new electron acceptor perylene diimide molecules for photovoltaic applications (2013) Dyes and Pigments, 99 (2), pp. 329-338. DOI: 10.1016/j.dyepig.2013.05.011

21) Kozma, E., Kotowski, D., Luzzati, S., Catellani, M., Bertini, F., Famulari, A., Raos, G. Improving the efficiency of P3HT:perylene diimide solar cells via bay-substitution with fused aromatic rings (2013) RSC Advances, 3 (24), pp. 9185-9188. DOI: 10.1039/c3ra41574k

22) Chiappe, C., Sanzone, A., Mendola, D., Castiglione, F., Famulari, A., Raos, G., Mele, A. Pyrazolium- versus imidazolium-based ionic liquids: Structure, dynamics and physicochemical properties (2013) Journal of Physical Chemistry B, 117 (2), pp. 668-676. DOI: 10.1021/jp3107793

23) A. Famulari, G. Raos, A. Baggioli, M. Casalegno, R. Po, S.V. Meille "A Solid State Density Functional Study of Crystalline Thiophene-Based Oligomers and Polymers" JOURNAL OF PHYSICAL CHEMISTRY. B, CONDENSED MATTER, MATERIALS, SURFACES, INTERFACES & BIOPHYSICAL 116, 14504-14509 (2012).

24) Polino, D., Famulari, A., Cavallotti, C. Analysis of the reactivity on the c7h6 potential energy surface (2011) Journal of Physical Chemistry A, 115 (27), pp. 7928-7936. DOI: 10.1021/jp2019236

25) Buono, A., Famulari, A., Meille, S.V., Ricci, G.L., Porri, L. 2,3-Exo-disyndiotactic polynorbornene: A crystalline polymer with tubular helical molecular structure annamaria (2011) Macromolecules, 44 (10), pp. 3681-3684. DOI: 10.1021/ma200490d