Fabio Capone

Drug Discovery Lab

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RESEARCH INTEREST AND SCIENTIFIC ACTIVITY

Since the beginning of Master Degree thesis, I am focused on interdisciplinary and integrated strategies involving in silico studies. Ab-initio modeling of periodic systems and surface adsorption were the first research interests. During Ph.d studies I investigated molecular dynamics model of amorphous systems.

Work Experience

- **Research Fellow**
  1th June 2017 – 31th January 2018
  Dept. of Pharmacy
  University of Naples Federico II
  Research activity: AB INITIO AND MOLECULAR DYNAMICS STUDIES OF NEW POTENTIAL LIGANDS OF PEROXISOME-PROLIFERATOR-ACTIVATED RECEPTORS

- **Honorary fellowship in Drug Analisys**
  1th May 2016 – now
  Dept. of Pharmacy
  University of Naples Federico II
  Professor: Prof. A Lavecchia

Education

- **Ph.d in Materials and Structures Engineering**
  30th April 2016
  Supervisor: Prof. Mauro Causà
  Thesis: THERMODYNAMICS OF POLYCAPROLACTONE-WATER SYSTEMS ANALYSIS OF INTERACTIONAL ISSUES BY COMPARING AB-INITIO AND MOLECULAR APPROACHES WITH A CLASSICAL LATTICE FLUID THEORY OF MIXTURES

- **Master's Degree, Chemistry**
  13th December 2012
  Supervisor: Prof. Vincenzo Busico
  Thesis: A THEORETHICAL APPROACH TO HETEROGENEOUS CATALYSIS: MODELS OF DONORS ADSORPTION ON $MGCL_2$ SURFACES

- **Bachelor's Degree, Chemical Sciences**
  21th December 2009
  Supervisor: Prof. Claudio De Rosa

Key Skills

- Languages
  Italian (mother tongue)
  English (fluent)

- Digital competence
  OS Linux proficient user
  Serial and parallel programming experties (FORTRAN90,Python,R)
  Attendance at CINECA course “Introduction to Parallel computing with MPI and OpenMP”

- Software of relevance in Computational Physical Chemistry
  ab-initio calculations: GAMESS-US, CRYSTAL14
  molecular mechanics: AMBER, NAMD, DLPOLY
  drug discovery: Maestro, GOLD, AutoDock Vina

Peer-reviewed Publications

1. Periodic Hybrid DFT Approach (Including Dispersion) to MgCl2-Supported Ziegler–Natta Catalysts. 2. Model Electron Donor Adsorption on MgCl2 Crystal Surfaces
F Capone, L Rongo, M D'Amore, PHM Budzelaar, V Busico
The Journal of Physical Chemistry C 117 (46), 24345-24353 22 **2013**

2. Orthogonal H-bonding synthons, actual and virtual structures in molecular crystals: a case study
R Centore, M Causà, F Cerciello, **F Capone**, S Fusco
CrystEngComm 16 (39), 9168-9175 3 **2014**

3. Competition between Polar and Centrosymmetric Packings in Molecular Crystals: Analysis of Actual and Virtual Structures
R Centore, S Fusco, **F Capone**, M Causà
Crystal Growth & Design 16 (4), 2260-2265 2 **2016**

4. Structure-Based Design, Synthesis and in vivo Antinociceptive Effects of Selective A1 Adenosine Receptor Agonists
R Petrelli, M Scortichini, C Belardo, S Boccella, L Luongo, **F Capone**, S Kachler, P Vita, F Del Bello, S Maione, A Lavecchia, K Klotz, L Cappellacci
Journal of medicinal chemistry **2017**

5. Novel Benzylidene Thiazolidinedione Derivatives as Partial PPARγ Agonists and their Antidiabetic Effects on Type 2 Diabetes
S Yasmin, **F Capone**, A Laghezza, F Dal Piaz, F Loiodice, V Vijayan, V Devadasan, S K Mondal, Ö Atlı, M Baysal, A K Pattnaik, V Jayaprakash, A Lavecchia
Scientific Reports 7 (1), 14453 **2017**

Interests

I enjoy mountaineering and speleology and I am a member of the Club Alpino Italiano (CAI). The latter involved cultural/promotional events and activities. I also enjoy current affairs and travelling.