Michele Aparecida Salvador, DSc.

Curriculum Vitae

Name Michele Aparecida Salvador

Nationality Brazilian

ORCID ID 0000-0002-8631-5702

Current Position Post doctoral researcher at Dipartimento di Scienze Matematiche Fisiche e Informatiche, University of Modena and Reggio Emilia

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Educational Experience

2009 - 2014 **Doctorate Degree (Dsc.), Nanosciences and Advanced Materials.**
Universidade Federal do ABC (UFABC), Santo Andre, Brazil
Thesis: Monte Carlo simulation of magnetic fluis onto magnetoliposomes.
Supervisor: Prof Dsc. Ronei Miotto;
Major tasks: Developed and adapted algorithms which allowed to study the behavior and properties of magnetic uids and magnetoliposomes, using computational tools to understand the role of physical and chemical variables, to characterize and predict the evolution of such systems.

2007 - 2009 **Master Degree (Msc.), Materials Engineering.**
Universidade Federal de Ouro Preto (UFOP), Ouro Preto, Brazil
Thesis: Surface Analyses of polymer thin lms using image processing tools.";
Supervisor: Andrea Gomes Campos Bianchi
Major tasks: Studied morfological properties of polymer thin films using image processing tools.

2003 - 2006 **Bachelor in Physics.**
Universidade Federal de Ouro Preto (UFOP), Ouro Preto, Brazil

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Research Experience

2021 - Post-doctorate.
University of Modena and Reggio Emilia, Modena, Italy.

Major tasks: Used molecular modelling to undestand inferface phenomena in polymer electrolytes.

2018 - 2020 Post-doctorate.
Universidade de São Paulo (USP), Sao Paulo, Brasil
Funding: PETROBRAS
Major tasks: Used multiscale molecular modelling to undestand the enhanced oil recovery process.

2015 - 2017 Post-doctorate.
Universidade Federal do ABC (UFABC), Santo Andre, Brazil
Funding: Conselho Nacional de Desenvolvimento Científico e Tecnológico;
Major tasks: Used the combination of classic (molecular dynamics and Monte Carlo) and quantum (DFT, semi-empirical) methodologies to model nanostructured sensors used in the detection of pharmaceutical drugs.

Additional Coursework

2017 *Atomic Scale Simulations.* (short course - 40 hours), Federal University of ABC (UFABC), Brazil;

2016 *Escuela de simulación computacional en ciencias de materiales. (short course - 80 hours),* Universidad de Buenos Aires (UBA), Argentina.

2011 *VIII Brazilin School o f Magnetism.* Physics Brazilian Society (SBF), Brazil.

2011 *Nanotechnology on therapeutics* (short course, 80 hours) Centro Brasileiro-Argentino de Nanotecnologia (CBAN), Brazil.

Professional Experience

2018 Online tutoring in specialization course “Nascimento e desenvolvimento da Ciência e seus desdobramentos para a contemporaneidade". Universidade Federal do ABC (UFABC).

2014 Temporary Professor, teaching Mathematics and Physics classes for undergraduate courses of Administration and Mecanical Engineering. Universidade São Francisco (USF).

Extracurricular Activities

2018 Volunteer work teaching Physics and Mathematic classes for high-school students in preparatory courses for college;

2018 – 2020 Collaborator at “Guia dos Entusiastas da Ciência” science communication project and blog;

Publications

1. Papers

1. **Salvador, Michele A.**; Antonio, Felipe C. T.; Silva, Gabriela D.; Bartoloni, F. H.; Orestes, E.; Coutinho, Maurício D.; Homem-De-Mello, P. *On The Radicalar Properties Of Graphene Fragments: Double-Hybrid DFT and Perturbation Theory Approaches.* Theoretical Chemistry Accounts. , V.139, P.118 - , 2020.

2. Da Silva, Gabriela Dias; De Freitas Martins, Ernane; **Salvador, Michele Aparecida**; Baptista, Alvaro David Torrez; De Almeida, James Moraes; Miranda, Caetano Rodrigues; From Atoms to Pre-salt Reservoirs: Multiscale Simulations of the Low-Salinity Enhanced Oil Recovery Mechanisms. Polytechnica. , v.26, p.30 - 50, 2019.

3. **Salvador, Michele A.**; Sousa, Camila P.; Maciel, Cleiton D.; Gomes, Rayane N.; Morais, Simone; De Lima-Neto, Pedro; Coutinho-Neto, Maurício D.; Correia, Adriana N.; Homem-De-Mello, Paula; Experimental and computational studies of the interactions between carbon nanotubes and ionic liquids used for detection of acetaminophen. SENSORS AND ACTUATORS B-CHEMICAL. , v.277, p.640 - 646, 2018.

4. Lima, Thays Souza; A. La-Scalea, Mauro; Raminelli, Cristiano; Simões, Fábio R.; Franco, Edison; Da Silva, Gabriela Dias; **Salvador, Michele Aparecida**; Homem-De-Mello, Paula; De Oliveira, Hueder P. M.; Codognoto, Lúcia; Voltammetric determination of chlorothalonil and its respective reduction mechanism studied by density functional theory. JOURNAL OF SOLID STATE ELECTROCHEMISTRY. , v.23, p.553 - 563, 2018.

5. Sousa, Camila P.; De Oliveira, Raissa C.; Freire, Tiago. M.; Fechine, Pierre B.A.; **Salvador, Michele A.**; Homem-De-Mello, Paula; Morais, Simone; De Lima-Neto, Pedro; Correia, Adriana N.; Chlorhexidine digluconate on chitosan-magnetic iron oxide nanoparticles modified electrode: Electroanalysis and mechanistic insights by computational simulations. Sensors and Actuators. B, Chemical. , v.240, p.417 - 425, 2017.

6. Sousa, Camila P.; **Salvador, Michele A.**; Homem-De-Mello, Paula; Ribeiro, Francisco W.P.; De Lima-Neto, Pedro; Correia, Adriana N.; Computational modeling of functionalized multi-walled carbon nanotubes dispersed in polyethylenimine for electrochemical sensing of acetaminophen. SENSORS AND ACTUATORS B-CHEMICAL. , v.246, p.969 - 978, 2017.

7. **Salvador, Michele Aparecida**; Sousa, Camila Pinheiro; Morais, Simone; Lima-Neto, Pedro De; Correia,

Adriana Nunes; Homem-De-Mello, Paula; Evaluation of Degradation Mechanism of Chlorhexidine by means of Density Functional Theory Calculations. COMPUTATIONAL BIOLOGY AND CHEMISTRY. , v.71, p.82 - 88, 2017.

8. **Salvador, Michele Aparecida**; Costa, Anderson Silva; Gaeti, Marilisa; Mendes, Livia Palmerston; Lima, Eliana Martins; Bakuzis, Andris Figueiroa; Miotto, Ronei; Characterization, nanoparticle self-organization, and Monte Carlo simulation of magnetoliposomes. PHYSICAL REVIEW E. , v.93, p.022609/1 - 14, 2016.
9. **Salvador, Michele A.**; Bianchi, Andrea G.C.; Pereira-da-Silva, Marcelo A.; Carvalho, Antonio J.F.; Faria, Roberto M. Dynamic formation of SEBS copolymer submicrometric structures. POLYMER. , v.51, p.4145 - 4151, 2010.

2. Book

1. Aono, C. M.; Silva, G. D.; Milani, C.; Vieira, C. R.; Maciel, C. D.; Liandra-Salvador, E.; Carvalho, F.; Kato, F. H.; Antonio, F. C. T.; Souza, L. R.; Zanotto, M.; **Salvador, M. A.**; Augusto, P.; Alvim, R. S.; Fernandes, V.; Alberto-Silva, C.; Rodrigues, M. G.; Souza-Garcia, J.; Homem-De-Mello, P.; Professor, para que estudo isso?. São Paulo: Livraria da Física, 2017, v.1. p.188.

3. Book Chapter

1. Liandra-Salvador, E.; Antonio, F. C. T.; Carvalho, F.; Franco-Junior, E.; Souza-Garcia, J.; **Salvador, M. A.**; Miotto, Ronei; Homem-De-Mello, P.; Moléculas Brilhantes In: Contém Química: A leitura deste livro pode causar dependência.1 ed.São Bernardo do Campo: EdUFABC, 2016, v.1, p. 29-56.

4. Conference Papers

1. Baptista, Alvaro David Torrez; **Salvador, Michele Aparecida**; Silva, Gabriela Dias Da; Martins, Ernane De Freitas; Almeida, James Moraes De; Miranda, Caetano Rodrigues; Multiscale Coupling between Molecular Simulations and Reservoir Simulator: Geochemical Reactions for Low Salinity Water Injection in Carbonates In: Offshore Technology Conference Brasil, 2019, Rio de Janeiro. **Offshore Technology Conference Brasil**. , 2019.

2. Martins, Ernane De Freitas; Da Silva, Gabriela Dias; **Salvador, Michele Aparecida**; Baptista, Alvaro David Torrez; De Almeida, James Moraes; Miranda, Caetano Rodrigues; Uncovering the Mechanisms of Low-Salinity Water Injection EOR Processes: A Molecular Simulation Viewpoint In: Offshore Technology Conference Brasil, 2019, Rio de Janeiro. **Offshore Technology Conference Brasil**. , 2019.

Language skills: Portuguese (native speaker), English (proficient).

Research skills: Molecular Modeling tools for Quantum (Gaussian, Orca, Quantum ESPRESSO, VASP) and Classical (Gromacs, Amber, LAMMPS) simulations. Computer simulation tools as FORTRAN, MATLab, etc. Knowlege in simulation methods as Monte Carlo.

Areas of interest: Condensed Matter Physics, Materials Engineering, Nanosciences and Nanotechnology, Theoretical Chemistry, Molecular Modeling.
