GRADUATE COURSE

Instituto de Química, Universidade de São Paulo,
São Paulo, SP, Brazil

QFL5648: "INTRODUCTION TO SIMULATION TECHNIQUES OF PHOTOPHYSICAL AND PHOTOCHEMICAL PROCESSES IN BIOLOGICAL ENVIRONMENTS"

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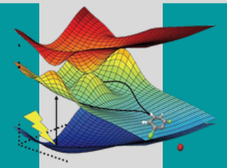
February 2022



GRADUATE COURSE
COMPUTATIONAL PHOTOCHEMISTRY

IQ - USP

ORGANIZATION AND INFORMATION:
Prof. Dr. Antonio Carlos Borin

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São Paulo, SP, Brazil
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LANGUAGE:
Lectures in English

NOTES and REMARKS:
Theoretical and practical classes;
All lectures will be online.
08 credits for USP students
and
Students of others institutions (inscrition form)

The course will also be broadcast live on
YouTube channel allowing participation via chat.

OBJECTIVES:

An introduction to fundamental aspects of hybrid quantum chemical methods (quantum chemistry and molecular mechanics, QM/MM) and applications in photochemistry and photophysics of biological systems.

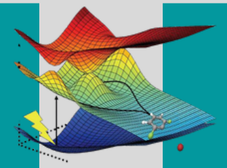
CONTENT:

This course will be an introduction to the theoretical chemistry methods usually employed to model physical and chemical processes taking place in biological environments: classical molecular dynamics, enhanced-sampling techniques, such as umbrella sampling and gaussian accelerated molecular dynamics, and QM/MM schemes for both ground and excited states. The methods will be explained in theory lectures and will be applied to practical problems in hands-on sessions.

ASSESSMENT:

Discussions about selected material from the literature.

QFL5648



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SCHEDULE:

1) Theoretical classes: 12 hours (4 days, 3 hours per class):
   a) February 01 (Tuesday): 10:00 - 13:00
   b) February 04 (Friday): 10:00 – 13:00
   c) February 08 (Tuesday): 10:00 - 13:00
   d) February 11 (Friday): 10:00 – 13:00

2) Computacionais practical classes with free software: AmberTools, Orca, VMD, MoBioTools): 16 hours (4 days, 4 hours per class):
   a) February 15 (Tuesday): 9:00 – 13:00
   b) February 18 (Friday): 9:00 – 13:00
   c) February 22 (Tuesday): 9:00 – 13:00
   d) February 25 (Friday): 9:00 – 13:00

BIBLIOGRAPHY:

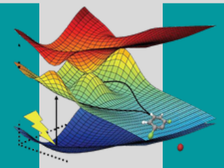
1. J. J. Nogueira and L. González. Annu. Rev. Phys. Chem. 2018, 69, 473.
2. E. Brunk and U. Rothlisberger. Chem. Rev. 2015, 115, 6217.
3. S. A. Adcock and J. A. McCammon. Chem. Rev. 2006, 106, 1589.
4. C. D. Christ, A. E. Mark, and W. F. van Gunsteren. J. Comput. Chem. 2010, 31, 1569.
5. MoBioChem group YouTube channel. https://www.youtube.com/c/MoBioChem

QFL5648

PROGRAM:

Theory Lectures 10:00 – 13:00:

- Day 1. 1st Feb 2022: Molecular Dynamics, Equations of Motion and Force Fields (https://youtu.be/bSnwWyzOP4c)
- Day 2. 4th Feb 2022: Periodic Boundary Conditions. Introduction to Enhanced-Sampling Approaches (https://youtu.be/g_wrYUKNyc4)
- Day 3. 8th Feb 2022: Umbrella Sampling and Replica Exchange (https://youtu.be/A3SxYkoKInM)
- Day 4. 11th Feb 2022: QM/MM and Research Examples (https://youtu.be/lgezhl719no)



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Computer Exercises 9:00 – 13:00
Software: AmberTools, Orca, VMD, MoBioTools

- Day 5. 15th Feb 2022: Classical Molecular Dynamics (https://youtu.be/cHpqEkMru3A)
- Day 6. 18th Feb 2022 :Umbrella Sampling (https://youtu.be/dvo6noErrbc)
- Day 7. 22nd Feb 2022: Computation of Redox Potentials (https://youtu.be/NRpnKUJXA7E)
- Day 8. 25th Feb 2022: Computation of Absorption Spectra (https://youtu.be/IsR5i8Na1wg)

QFL5648

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