

# Webinars on Computational Photochemistry

"Understanding Isomerization - Insight from Hybrid QM/MM Molecular Dynamics Simulations"

[Dr. Igor Schapiro](#)

The Hebrew University of Jerusalem, Israel

November 27, 2020 (Friday) **11am (BRT time)**

Google Meet

Organization: [Prof. Dr. Antonio Carlos Borin](#)

[Instituto de Química, Universidade de São Paulo \(USP\), SP, Brazil](#)

Information and Registration: [ancborin@iq.usp.br](mailto:ancborin@iq.usp.br)

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With the words "Igor Schapiro – Virtual" on the "subject"

Deadline: November 25, 2020 (Wednesday), 06pm (BRT time).



# Understanding Isomerization – Insight from Hybrid QM/MM Molecular Dynamics Simulations

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The primary event of vision in the vertebrate eye is the highly selective and efficient photoisomerization of 11-cis-retinal protonated Schiff base (RPSB) bound to the visual protein rhodopsin (Rh). With a ~100% selectivity, ~65% quantum yield, and ~200 fs product appearance time, this isomerization is considered the archetype of a photochemical reaction optimized by nature to achieve a specific molecular response.

Recently, we have used a combination of a quantum chemical and a classical force field method (QM/MM) to resolve the isomerization mechanism for the RPSB chromophore in Rh[1].

Important stereoelectronic factors were found that determine the outcome of the photoisomerization.[2] The same protocol was also applied to study the ground state (thermal) isomerization.[3] The results of the simulations explain the molecular mechanism of thermal noise in rod photoreceptors and make a direct link to experimentally found correlations for night vision.

## References:

- [1] Schapiro I, Ryazantsev M N, Frutos L M, Ferré N, Lindh R, Olivucci M. J. Am. Chem. Soc. (2011) 133, 3354.
- [2] Schnedermann C, et al. Nature Chemistry (2018) 10, 449.
- [3] Gozem S, Schapiro I, Ferré N, Olivucci M. Science (2012) 33, 6099.