Sanibel Symposium

Flyer

65th Sanibel Symposium

The Theory Meeting for Theoreticians

St. Augustine Beach, FL

Feb 22nd – Feb 27th, 2026

Please join us for the Sanibel meeting at St. Augustine Beach!!!

The largest annual meeting in the quantum theory of atoms, molecules and materials will take place at the Embassy Suites Hotel in St. Augustine Beach, FL. The Sanibel Meeting emphasizes developments in the fields of quantum molecular and material science.

The 2026 meeting will feature various topics dealing with theoretical developments and their role in molecules, materials, computational and information science. Many of these new developments will build upon themes that have been nurtured by the influence of the Sanibel meeting in the fields, and presentations will be made by a broad array of experts. Topics addressed in the lectures will include those listed below:

- John F. Stanton Memorial
  - Correlated System Methods beyond Coupled Cluster
  - Chirality in Quantum Chemistry
  - 2D Moire Systems
  - Quantum dynamics of molecules and materials
  - Quantum Computing
  - Quantum methods for electrochemistry

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Beyond these sessions and evening poster presentations, Sanibel offers slots for competitively selected 'hot-topic' talks that makes it possible for all attendees to present their work comfortably while benefiting from the valuable feedback offered by the Sanibel attendees.

Registration: https://sanibelsymposium.qtp.ufl.edu/registration/

Early registration ends: **November 30th, 2025**

Award applications must be submitted before **January 19th, 2026**

Abstract Submission Deadline: January 19, 2026. (Latest for print is 1/23/26) the link will be open for late submissions:

Https://sanibelsymposium.qtp.ufl.edu/abstract-submission/

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Hydrogen Bonds as Key Drivers of Stability and Electronic Spectra in Sulfapyridine Tautomers

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Sulfapyridine (SPY) is an antibiotic widely used in medicine and livestock/aquaculture that is frequently associated with contamination of aquatic environments.[1] In a recent work, we probed the effects of microsolvation on the tautomerization mechanism of SPY under different pH conditions. Here, we focus on understanding the role of hydrogen-bond interactions in the stabilization and electronic absorption spectra of SPY tautomers at different pH values. Previously, the presence of two explicit water molecules rendered the tautomeric form of SPY (TAUT) the most stable one in neutral and acidic media (−1.28 and −2.79 kcal·mol^{-1}), in addition to decreasing the tautomerization barrier heights. Thus, we applied the Quantum Theory of Atoms in Molecules (QTAIM)[2] to evaluate the electronic density (ρ), Laplacian of the electronic density ($\nabla^2\rho$), energy density (H), electronic localization function (ELF), ellipticity (ε), and potential energy density (V), in order to investigate the stabilization of the TAUT form under both pH conditions. Time-dependent DFT (TD-DFT) was employed to obtain the electronic absorption spectra of these species. In general, the QTAIM analysis revealed that cooperative hydrogen bonds are responsible for the stabilization of the TAUT form. Furthermore, the Espinosa relation,[3] used to estimate the stabilization energy from the network of hydrogen bonds, is in agreement with the relative Gibbs free energies obtained previously. For example, the network of hydrogen bonds in the neutral TAUT form is 1.31 kcal·mol^{-1} more stable than that in the SPY form. TD-DFT calculations with implicit solvation are in good agreement with experimental spectra.

References

[1]Duan, W.; Cui, H.; Jia, X.; Huang, X. *Sci. of The Tot. Environ.* **2022**, 820, 153178.

[2]Bader, R.F.W. *Accounts of Chemical Research*, **1985**, 18(1), 9-15.

[3]Espinosa, E., Molins, E. and Lecomte, C. *Chem. Phys. Letters*, **1998**, 285(3-4), 170-173.