Mikołaj Martyka

Lista Publikacji

1. Martyka M., Zhang L., Ge F., Hou Y-F., Jankowska J., Barbatti M., Dral. P. O. (2025) Charting electronic-state manifolds across molecules with multi-state learning and gap-driven dynamics via efficient and robust active learning. npj Computational Materials, 11, (1), artykuł nr 132.

2. Martyka M., Jankowska J. (2023) Nonadiabatic molecular dynamics study of a complete photoswitching cycle for a full-size diarylethene system. Journal of Photochemistry and Photobiology A: Chemistry, 438, 114513.

3. Martyka M., Jankowska J. (2024) New insights into the photocyclization reaction of a popular diarylethene switch: a nonadiabatic molecular dynamics study. Physical Chemistry Chemical Physics, 26 (16), 13383-13394.

4. Martyka M., Jankowska J. (2025) Polarized molecular wires for efficient photo-generation of free electric charge carriers. Physical Chemistry Chemical Physics, 27 (11), 5631-5640.

5. Zhang L., Pios S. V., Martyka M., Ge F., Hou Y-F., Chen Y., Chen L., Jankowska J., Barbatti M., Dral P. O. (2024) MLatom software ecosystem for surface hopping dynamics in Python with quantum mechanical and machine learning methods. Journal of Chemical Theory and Computation, 20 (12), 5043-5057.