



Julia WESTERMAYR



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Supervisor: Leticia González,
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Thesis title: Machine Learning
for Excited-State Molecular
Dynamics Simulations.

Current Position: “Erwin
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MolTag alumni page:

[Julia Westermayr \(univie.ac.at\)](https://univie.ac.at)

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How would you summarize your thesis results in 3 sentences?

I developed machine learning models to investigate photo-initiated reactions. Due to the computational efficiency of machine learning, simulations could be speed up such that better statistics and long time scale molecular dynamics simulations were achieved. The developed method was applied to small molecules.

What was the impact of the MolTag program on your further career?

The MolTag program **helped me a lot in communicating with researchers from different disciplines**, i.e., it improved my communication as a theoretician with experimental scientists. The interdisciplinary activities and the discussions/talks we had to explain our research to others were definitely helpful. Furthermore, the **tips for our future career of SAB members and PIs helped me a lot in deciding on the next steps after my PhD.**

Did you keep connections with some former colleagues?

Yes, especially because I plan to come back to Vienna for one year due to a fellowship I received.

What did you particularly like about the MolTag program?

I liked the fact that **it brings together scientists from different disciplines who might not have met without this program.** I especially enjoyed the research internship at the lab of one of the SAB members, where I could learn about simulations of metalloproteins.

What is your recommendation for the MolTag PhD students?

Never compare yourself to others – in performance, number of publications, etc. Always remember that you are the only one who knows most about your project, that you are the most suitable person to solve related problems. No doctoral thesis is similar to another.

